

Functional Regression with Unknown Manifold Structures

Zhenhua Lin

Department of Statistical Sciences, University of Toronto, Toronto, Canada.

E-mail: zhenhua@utstat.toronto.edu

Fang Yao

Department of Statistical Sciences, University of Toronto, Toronto, Canada.

E-mail: fyao@utstat.toronto.edu

Summary. Statistical methods that adapt to unknown population structures are attractive due to both practical and theoretical advantages over their non-adaptive counterparts. We contribute to adaptive modelling of functional regression, where challenges arise from the infinite dimensionality of functional predictor in the underlying space. We are interested in the scenario that the predictor process lies in a potentially nonlinear manifold that is intrinsically finite-dimensional and embedded in an infinite-dimensional functional space. By a novel functional regression approach built upon local linear manifold smoothing, we achieve a polynomial rate of convergence that adapts to the intrinsic manifold dimension and the level of noise/sampling contamination with a phase transition phenomenon depending on their interplay, which is in contrast to the logarithmic convergence rate in the literature of functional nonparametric regression. We demonstrate that the proposed method enjoys favourable finite sample performance relative to commonly used methods via simulated and real data examples.

Keywords: Contaminated functional data, functional nonparametric regression, intrinsic dimension, local linear manifold smoothing, phase transition

1. Introduction

Regression with a functional predictor is of central importance in the field of functional data analysis, the field that has been advanced by Ramsay and Silverman (1997) and Ramsay and Silverman (2002),

among other researchers. Early development of functional regression focuses on functional linear models, such as Cardot et al. (1999), Cardot et al. (2003), Yao et al. (2005b), Hall and Horowitz (2007), and Yuan and Cai (2010). Extensions of linear models include generalized linear regression by Cardot and Sarda (2005) and Müller and Stadtmüller (2005), additive model by Müller and Yao (2008), quadratic model by Yao and Müller (2010), among many others. These works prescribe some specific forms of the regression model, and may be regarded as functional “parametric” regression models (Ferraty and Vieu, 2006) which often entail an efficient estimation procedure and hence are well studied in the literature.

In contrast, functional “nonparametric” regression that does not impose structural constraints on the regression function receives relatively less attention. The first landmark development of nonparametric functional data analysis is the monograph of Ferraty and Vieu (2006). Recent advances on functional nonparametric regression include Nadaraya-Waston estimator studied by Ferraty et al. (2012), and k -nearest-neighbor (k NN) estimators investigated by Kudraszow and Vieu (2013). The development of functional nonparametric regression is hindered by a theoretical barrier that is formulated in Mas (2012) and is linked to the small ball probability problem (Delaigle and Hall, 2010). Essentially, it was shown that in a rather general setting, the minimax rate of nonparametric regression on a generic functional space is slower than any polynomial of sample size, as opposite to functional parametric regression (e.g. Hall and Horowitz, 2007; Yuan and Cai, 2010, for functional linear regression). These endeavours on functional nonparametric regression do not explore the intrinsic structures that are not uncommon in practice. However, Chen and Müller (2012) suggests that functional data often possess a low-dimensional manifold structure and demonstrates that such structures can be utilized for more efficient representation. By contrast, in this work we consider to explore *nonlinear* low-dimensional structures for functional nonparametric regression.

Specifically, we study the following model,

$$Y = g(X) + \varepsilon, \tag{1}$$

where Y is a scalar response, X is a functional predictor sampled from an unknown manifold \mathcal{M} , ε is the error term that is independent of X , and g is some unknown functional that is to be

estimated. This model features a manifold structure \mathcal{M} that underlies the functional predictor X and is embedded in the functional space $\mathcal{L}^2(D)$, the space of square integrable functions defined on a compact domain $D \subset \mathbb{R}$. For a background on manifold, we refer readers to Lang (1995) and Lang (1999). Although data analysis with manifold structures has been studied in the statistical literature (e.g., Yuan et al., 2012; Cornea et al., 2016), the literature relating functional data to manifolds is scarce. Chen and Müller (2012) considers the representation of functional data on a manifold that has only one chart and hence is essentially a linear manifold. Zhou and Pan (2014) investigates functional principal component analysis on an irregular planar domain which can be viewed as a linear manifold as well. Mostly related to our work is Lila and Aston (2017) that models functions sampled from a nonlinear two-dimensional manifold and focuses on the principal component analysis. To the best of our knowledge, we are the first to consider a nonlinear manifold structure in the setting of functional regression where a *global* representation of X living in a nonlinear low-dimensional can be inefficient.

For illustration, in Example 1, we give a *one-dimensional* manifold embedded in $\mathcal{L}^2([0, 1])$, and a random process X taking value in this manifold, where X has an *infinite* number of components in its Karhunen-Loève expansion. By contrast, the *local* Karhunen-Loève expansion of X within a small neighborhood of a given $x \in \mathcal{M}$ provides sufficient information about the tangent space at x and can be used to construct a local linear estimate for g at x , as described in Section 3.2.

EXAMPLE 1. Let $S^1 = \{v(\omega) = (\cos 2\pi\omega, \sin 2\pi\omega) : \omega \in [0, 1]\}$ denote the unit circle. It is a one-dimensional manifold. Denote ϕ_1, ϕ_2, \dots a complete orthonormal basis of $\mathcal{L}^2([0, 1])$. Define a map $X(v(\omega)) = \sum_k k^{-c} \cos(2k\pi\omega) \phi_k$ with $c > 3/2$. Then X is an immersion. Since S^1 is compact, X is also an embedding, and the image $X(S^1)$ is an embedded manifold in $\mathcal{L}^2([0, 1])$. We show that the embedded tangent space at $v(\omega)$ is $\text{span}\left\{\sum_k k^{-c} 2k\pi \sin(2k\pi\omega) \phi_k\right\}$, see Section S.1 in the Supplementary Material for derivation. If we treat $[0, 1]$ as a probability space endowed with the usual Lebesgue measure, and define random variables $\xi_k(\omega) = k^{-c} \cos(2k\pi\omega)$. Then $X = \sum_k \xi_k \phi_k$ can be regarded as a random process. It is easy to check that $\mathbf{E}(\xi_k \xi_j) = 0$ if $k \neq j$, $\mathbf{E}(\xi_k) = 0$, and $\mathbf{E}\xi_k^2 = k^{-2c}/2$, which implies that $\mathbf{E}(\|X\|_{\mathcal{L}^2}^2) < \infty$. One can see that the covariance operator of X has eigenvalues $\lambda_k = \mathbf{E}\xi_k^2 = k^{-2c}/2$ and corresponding eigenfunctions ϕ_k . Therefore, $X = \sum_k \xi_k \phi_k$

is the Karhunen-Loève expansion, which includes infinite number of components ξ_k , while X is intrinsically driven by merely a single parameter ω .

The approach we adopt to estimate the regression functional g in (1) is local linear manifold smoothing acting on tangent space, which was proposed by Cheng and Wu (2013) to study Euclidean type manifold regression. Despite of similar estimation methods, the problem we target at is materially different. First, we consider regression of functional data which naturally live in an infinite-dimensional space, while Cheng and Wu (2013) along with other researches on manifold learning in the literature, such as Bickel and Li (2007), considers manifolds embedded in Euclidean space. Second, we study the effect of noise/sampling contamination in the observed functional predictor on the regression. Unlike Cheng and Wu (2013) where the predictor is fully observed without noise, we observe its contaminated version to accommodate the realistic situations where functional data are measured intermittently and corrupted by noise. As a matter of fact, this type of contamination is distinct from the case of sparsely observed functional predictor (Yao et al., 2005b) and has not been well studied even in classical functional linear regression, e.g., Hall and Horowitz (2007) is based on fully observed functions and Kong et al. (2016) asymptotically ignores the error induced by pre-smoothing densely observed functions.

The main contributions of this article are as follows. First, by exploring structural information of the predictor, the proposed model entails an effective estimation procedure that adapts to the manifold structure and the contamination level while maintaining the flexibility of functional non-parametric regression. We stress that the underlying manifold is unknown, and we do not require *a priori* knowledge to construct our estimator. Second, we show that the regression functional g can be estimated at a polynomial convergence rate of the sample size, which innovates the theory of Mas (2012) that does not explore any intrinsic structure. Third, we discover that, the polynomial convergence rate exhibits a phase transition phenomenon, depending on the interplay between the intrinsic dimension of the manifold and the contamination level in the predictor. This type of phase transition in functional regression has not yet been studied, and is distinct from those concerning estimation of mean/covariance functions for functional data (e.g. Cai and Yuan, 2011; Zhang and Wang, 2016). In addition, during our theoretical development, we obtain some results

that are generally useful with own merit, such as the consistent estimation for the intrinsic dimension and the tangent spaces of the manifold that underlies the contaminated functional data, the convergence of an arbitrary moment in \mathcal{L}^2 difference for local linear estimation in the individual smoothing step.

We organize the rest of the paper as follows. In Section 2, we describe the estimation procedure. The theoretical properties of the proposed method are presented in Section 3. Numerical evidence via simulation studies is provided in Section 4, followed by real data examples in Section 5. Proofs of main theorems are deferred to the Appendix, while some auxiliary results and technical lemmas with proofs are placed in the online Supplementary Material for space economy.

2. Proposed Methodology

To estimate the functional g in model (1) based on an independently and identically distributed (i.i.d.) sample $\{(X_i, Y_i)\}_{i=1}^n$ of size n , we assume that each predictor X_i is observed at m_i design points $T_{i1}, T_{i2}, \dots, T_{im_i} \in D$. Here, we consider a random design of T_{ij} , where T_{ij} are i.i.d. sampled from a density f_T . We should point out that our method and theory in this article apply to the fixed design with slight modification. Denote the observed values at the T_{ij} by $X_{ij}^* = X_i(T_{ij}) + \zeta_{ij}$, where ζ_{ij} are i.i.d. random variables with mean zero and independent of all X_i and T_{ij} . Let $\mathbb{X}_i = \{(T_{i1}, X_{i1}^*), (T_{i2}, X_{i2}^*), \dots, (T_{im_i}, X_{im_i}^*)\}$, which represents all measurements for the realization X_i , and $\mathcal{X} = \{\mathbb{X}_1, \mathbb{X}_2, \dots, \mathbb{X}_n\}$ constitutes the observed data for the functional predictor.

We first recover each function X_i based on the observed data \mathcal{X} by individual smoothing estimation. Here we do not consider the case of sparsely observed functions when only a few noisy measurements are available for each subject (Yao et al., 2005a,b), due to the elevated challenge of estimating the unknown manifold structure, which can be a topic for further investigation. Commonly used techniques include local linear smoother (Fan, 1993) and spline smoothing (Ramsay and Silverman, 2005), among others. By applying any smoothing methods, we obtain the estimated \hat{X}_i of X_i , referred to as the contaminated version of X_i that are used in subsequent steps to estimate g at any given $x \in \mathcal{M}$. To be specific, we consider the local linear estimate of $X_i(t)$

given by \hat{b}_1 , where

$$(\hat{b}_1, \hat{b}_2) = \arg \min_{(b_1, b_2) \in \mathbb{R}^2} \frac{1}{n} \sum_{j=1}^{m_i} \{X_{ij}^* - b_1 - b_2(T_{ij} - t)\}^2 K\left(\frac{T_{ij} - t}{h_i}\right) \quad (2)$$

where K is a compactly supported density function and h_i is the bandwidth, leading to

$$\hat{b}_1 = \frac{R_0 S_2 - R_1 S_1}{S_0 S_2 - S_1^2}, \quad (3)$$

where for $r = 0, 1$ and 2 ,

$$S_r(t) = \frac{1}{m_i h_i} \sum_{j=1}^{m_i} K\left(\frac{T_{ij} - t}{h_i}\right) \left(\frac{T_{ij} - t}{h_i}\right)^r, \quad R_r(t) = \frac{1}{m_i h_i} \sum_{j=1}^{m_i} K\left(\frac{T_{ij} - t}{h_i}\right) \left(\frac{T_{ij} - t}{h_i}\right)^r X_{ij}^*.$$

One technical issue with the estimate (3) is the nonexistence of unconditional mean squared error (MSE, i.e., the expected squared \mathcal{L}^2 discrepancy), as the denominator in (3) is zero with a positive probability for finite sample. This can be overcome by ridging, as used by Fan (1993) and discussed in more details by Seifert and Gasser (1996) and Hall and Marron (1997). We thus use a ridged local linear estimate for $X_i(t)$

$$\hat{X}_i(t) = \frac{R_0 S_2 - R_1 S_1}{S_0 S_2 - S_1^2 + \delta 1_{\{|S_0 S_2 - S_1^2| < \delta\}}}, \quad (4)$$

where $\delta > 0$ is a sufficiently small constant depending on m_i , e.g., a convenient choice is $\delta = m_i^{-2}$.

To characterize the manifold structure for functional regression, we estimate the tangent space at the given x explicitly and then perform local linear smoothing on the coordinates $\hat{\mathbf{x}}_i$ of the observations \hat{X}_i when projected onto the estimated tangent space. To do so, we shall first determine the intrinsic dimension d of the manifold \mathcal{M} . We adopt the maximum likelihood estimator proposed by Levina and Bickel (2004), substituting the unobservable X_i with the contaminated version \hat{X}_i .

Denoting $\hat{G}_i(x) = \|x - \hat{X}_i\|_{\mathcal{L}^2}$ and $\hat{G}_{(k)}(x)$ the k th order statistic of $\hat{G}_1(x), \dots, \hat{G}_n(x)$, then

$$\hat{d} = \frac{1}{k_2 - k_1 + 1} \sum_{k=k_1}^{k_2} \hat{d}_k, \quad \text{with } \hat{d}_k = \frac{1}{n} \sum_{i=1}^n \hat{d}_k(\hat{X}_i), \quad \hat{d}_k(x) = \left\{ \frac{1}{k-1} \sum_{j=1}^{k-1} \log \frac{\hat{G}_{(k)}(x) + \Delta}{\hat{G}_{(j)}(x) + \Delta} \right\}^{-1}, \quad (5)$$

where Δ is a positive constant depending on n , and k_1 and k_2 are tuning parameters. Note that, in order to overcome the additional variability introduced by contamination, we regularize $\hat{d}_k(x)$ by an extra term Δ . We conveniently set $\Delta = 1/\log n$, while refer readers to Levina and Bickel (2004) for the choice of k_1 and k_2 . Given the estimate \hat{d} , we proceed to estimate the tangent space at the given point x as follows.

- A neighborhood of x is determined by a tuning parameter $h_{pca} > 0$, denoted by $\hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x) = \{\hat{X}_i : \|x - \hat{X}_i\|_{\mathcal{L}^2} < h_{pca}, i = 1, 2, \dots, n\}$.
- Compute the local empirical covariance function

$$\hat{\mathcal{C}}_x(s, t) = \frac{1}{|\hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)|} \sum_{\hat{X} \in \hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)} \{\hat{X}(s) - \hat{\mu}_x(s)\} \{\hat{X}(t) - \hat{\mu}_x(t)\} \quad (6)$$

using the data within $\hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)$ and obtain eigenvalues $\hat{\rho}_1 > \hat{\rho}_2 > \dots > \hat{\rho}_{\hat{d}}$ and corresponding eigenfunctions $\hat{\varphi}_1, \hat{\varphi}_2, \dots, \hat{\varphi}_{\hat{d}}$, where $\hat{\mu}_x = |\hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)|^{-1} \sum_{\hat{X} \in \hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)} \hat{X}$ is the local mean function and $|\hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)|$ denotes the number of observations in $\hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)$. This can be done by standard functional principal component analysis (FPCA) procedures, such as Yao et al. (2005a) and Hall and Hosseini-Nasab (2006).

- Estimate the tangent space at x by $\widehat{T_x \mathcal{M}} = \text{span}\{\hat{\varphi}_1, \hat{\varphi}_2, \dots, \hat{\varphi}_{\hat{d}}\}$, the linear space spanned by the first \hat{d} eigenfunctions.

Note that the eigen-decomposition of the function $\hat{\mathcal{C}}_x(s, t)$ provides a local Karhunen-Loève expansion of X at the given x which is used to construct an estimate of the tangent space at x . Finally, we project all \hat{X}_i onto the estimated tangent space $\widehat{T_x \mathcal{M}}$ and obtain coordinates

$\hat{\mathbf{x}}_i = (\langle \hat{X}_i, \hat{\varphi}_1 \rangle, \dots, \langle \hat{X}_i, \hat{\varphi}_{\hat{d}} \rangle)^T$. Then, the estimate of $g(x)$ is given by

$$\hat{g}(x) = \mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \mathbf{Y} \quad (7)$$

where

$$\hat{\mathbf{X}} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \hat{\mathbf{x}}_1 & \hat{\mathbf{x}}_2 & \cdots & \hat{\mathbf{x}}_n \end{bmatrix}^T,$$

$\hat{\mathbf{W}} = \text{diag}(K_{h_{reg}}(\|x - \hat{X}_1\|_{\mathcal{L}^2}), K_{h_{reg}}(\|x - \hat{X}_2\|_{\mathcal{L}^2}), \dots, K_{h_{reg}}(\|x - \hat{X}_n\|_{\mathcal{L}^2}))$ with $K_h(t) = K(t/h)/h^{\hat{d}}$ and the bandwidth h_{reg} , $\mathbf{Y} = (Y_1, Y_2, \dots, Y_n)^T$, and $\mathbf{e}_1^T = (1, 0, 0, \dots, 0)$ is an $n \times 1$ vector. The tuning parameter h_{reg} , along with h_{pca} , is selected by modified generalized cross-validation detailed in Cheng and Wu (2013). We emphasize that, in the above estimation procedure which is illustrated by a diagram in the top-left panel of Figure 1, all steps are based on the contaminated sample $\{\hat{X}_1, \dots, \hat{X}_n\}$, rather than the unavailable functions X_i .

3. Theoretical Properties

In this section, we investigate the theoretical properties of the estimate $\hat{g}(x)$ in (7). Recall that m_i denotes the number of measurements for the predictor X_i , we assume that m_i grows with sample size n at a polynomial rate. Without loss of generality, assume $m_i \asymp m \asymp n^\alpha$ for some constant $\alpha > 0$, where $a_n \asymp b_n$ denotes $0 < \liminf a_n/b_n < \limsup a_n/b_n < \infty$. The discrepancy between \hat{X}_i and X_i , quantified by $\|\hat{X}_i - X_i\|_{\mathcal{L}^2}$, is termed *contamination* of X_i . It turns out that, the decay of this contamination is intimately linked to the consistency of the estimates of the intrinsic dimension, the tangent spaces, and eventually the regression functional $g(x)$. As one of our main contributions, we discover that the convergence rate of $\hat{g}(x)$ exhibits a phase transition phenomenon depending on the interplay between the intrinsic dimension and the decay of contamination. In this section, the main results on functional regression are presented in Section 3.2, while the property of contamination in recovery of functional data is given in Section 3.1 to set the stage.

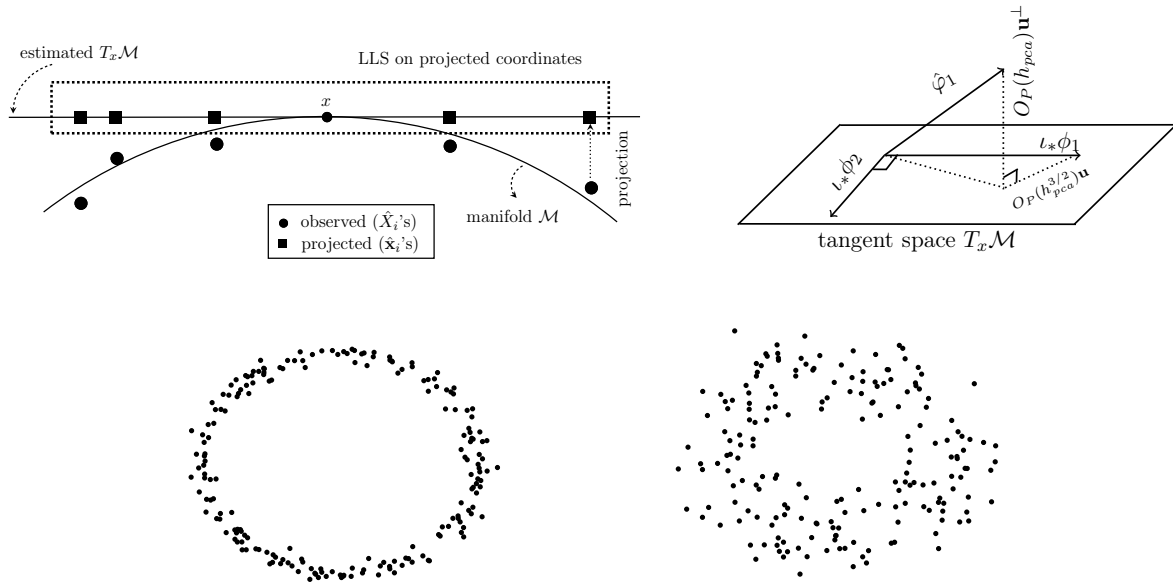


Fig. 1. Top left: illustration of functional regression on manifold; Top right: illustration of estimation quality of the tangent space at x ; Bottom left: 200 random samples from a unit circle with small noise where the structure of unit circle can be visually identified; Bottom right: 200 random samples from a unit circle with large noise where the structure is less obvious.

3.1. Contamination in smoothing functional data

Recall that the individual smoothing to recover each X_i is based on the measurements available for that individual, $\mathbb{X}_i = \{(T_{i1}, X_{i1}^*), (T_{i2}, X_{i2}^*), \dots, (T_{im}, X_{im}^*)\}$, so the estimates \hat{X}_i are also i.i.d., if the observed data are i.i.d., which simplifies our analysis and can be extended to weakly dependent \hat{X}_i without substantial changes. Specifically, we shall study the p th moment of contamination in \mathcal{L}^2 norm when \hat{X}_i is the ridged local linear estimate given by (4), while Fan (1993) derived the convergence rate of $\|\hat{X}_i - X_i\|_{\mathcal{L}^2}^2$ conditional on X_i . Let $\Sigma(\nu, L)$ denote the Hölder class with exponent ν and Hölder constant L_F , which represents the set of $\ell = \lfloor \nu \rfloor$ times differentiable functions F whose derivative $F^{(\ell)}$ satisfies $|F^{(\ell)}(t) - F^{(\ell)}(s)| \leq L_F |t - s|^{\nu - \ell}$ for $s, t \in D$, where $\lfloor \nu \rfloor$ is the largest integer strictly smaller than ν . We require mild assumptions as follows, and assume $h_i \asymp h_0$ without loss of generality.

- (A1) K is a differentiable kernel with a bounded derivative, $\int_{-1}^1 K(u) du = 1$, $\int_{-1}^1 uK(u) du = 0$, and $\int_{-1}^1 |u|^p K(u) du < \infty$ for all $p > 0$.
- (A2) The sampling density f_T is bounded away from zero and infinity, i.e., for some constants $C_{T,1}, C_{T,2} \in (0, \infty)$, $C_{T,1} = \inf_{t \in D} f_T(t) \leq \sup_{t \in D} f_T(t) = C_{T,2}$.
- (A3) $X \in \Sigma(\nu, L_X)$, where $L_X > 0$ is a random quantity and $0 < \nu \leq 2$ is some constant that quantifies the smoothness of the process.

THEOREM 1. *Suppose $h_0 \rightarrow 0$, and $mh_0 \rightarrow \infty$. For any $p \geq 1$, assume $\mathbf{E}|\zeta|^p < \infty$. Under assumptions (A1)–(A3), for the estimate \hat{X} in (4) with a proper choice of δ ,*

$$\{\mathbf{E}(\|\hat{X} - X\|_{\mathcal{L}^2}^p | X)\}^{1/p} = O\left(m^{-1/2} h_0^{-1/2}\right) \left\{ \sup_t |X(t)| + L_X \right\} + O(h_0^\nu) L_X, \quad (8)$$

where $O(\cdot)$ does not depend on X . With $h_0 \asymp m^{-\frac{1}{2\nu+1}}$, we have

$$\{\mathbf{E}(\|\hat{X} - X\|_{\mathcal{L}^2}^p | X)\}^{1/p} = O(m^{-\frac{\nu}{2\nu+1}}) \left\{ \sup_t |X(t)| + L_X \right\}. \quad (9)$$

It is interesting to note that the p th moment of the smoothing error does not depend on p . When X is deterministic as in nonparametric regression, the rate in (9) for $p = 2$ coincides that in

Tsybakov (2008). To obtain the the unconditional p th moment rate, assume that

$$(A4) \quad \text{for all } r \geq 1, \mathbf{E} \sup_t |X(t)|^r < \infty, \mathbf{E}(L_X)^r < \infty \text{ and } \mathbf{E}|\zeta|^r < \infty.$$

Note that $\mathbf{E} \sup_t |X(t)|^r < \infty$ holds rather generally, as discussed in Li and Hsing (2010); Zhang and Wang (2016), compared to a stronger assumption on X given in (A.1) of Hall et al. (2006). Then the following result is an immediate consequence of the theorem.

COROLLARY 1. *Under assumption (A1)–(A4), with $h_0 \asymp m^{-\frac{1}{2\nu+1}}$, we have*

$$\left(\mathbf{E} \|\hat{X} - X\|_{\mathcal{L}^2}^p \right)^{1/p} = O(m^{-\frac{\nu}{2\nu+1}}).$$

In addition, with $m \asymp n^\alpha$ for some $\alpha > 0$, we have

$$\left(\mathbf{E} \|\hat{X} - X\|_{\mathcal{L}^2}^p \right)^{1/p} = O(n^{-\frac{\alpha\nu}{2\nu+1}}).$$

The corollary shows that the p th order of the contamination $\|\hat{X}_i - X_i\|_{\mathcal{L}^2}$ decays at a polynomial rate which depends on the sampling rate α and smoothness of the process quantified by ν , but not the order of the moment p .

3.2. Convergence of estimated functional regression

Recall that \mathcal{M} is assumed to be embedded in $\mathcal{L}^2(D)$ in model (1). We use ι to denote the embedding which is also the inclusion map from \mathcal{M} to $\mathcal{L}^2(D)$. In the sequel, we use x and X to denote both $x, X \in \iota(\mathcal{M})$ and $\iota^{-1}(x), \iota^{-1}(X) \in \mathcal{M}$ when no ambiguity arises. To analyze the asymptotic property of $\hat{g}(x)$, we make following assumptions.

- (B1) The probability density f of X on \mathcal{M} satisfies $C_{f,1} = \inf_{x \in \mathcal{M}} f(x) \leq \sup_{x \in \mathcal{M}} f(x) = C_{f,2}$ for some constants $0 < C_{f,1} \leq C_{f,2} < \infty$.
- (B2) The regression functional g is twice differentiable with a bounded second derivative.
- (B3) $\hat{X}_1, \hat{X}_2, \dots, \hat{X}_n$ are independently and identically distributed. For some $\beta \in (0, \infty)$ and all $p \geq 1$, $\{\mathbf{E}(\|\hat{X} - X\|_{\mathcal{L}^2}^p \mid X)\}^{1/p} \leq C_p n^{-\beta} \eta(X)$ for some constant C_p depending only on p and some nonnegative function $\eta(X)$ depending only on X such that $\mathbf{E}\{\eta(X)\}^p < \infty$.

Note that the assumption (B3) is presented in terms of the contaminated predictor \hat{X} , and hence implicitly poses requirement for the smoothing method. Under assumptions (A1)–(A4), by Corollary 1, the individual smoothing via local linear estimation (4) satisfies (B3) with $\beta = \alpha\nu/(2\nu + 1)$. To give an intuitive interpretation, we define $\gamma = \beta^{-1} = (2 + \nu^{-1})/\alpha$ as the contamination level of \hat{X} . We see that the contamination level is low for densely observed (i.e., large α) or smoother (i.e., large ν) functions. We emphasize that our theory on estimated regression functional \hat{g} does not depend the smoothing method used in recovering X_i , as long as (B3) is fulfilled. Further, we may extend (B3) to allow weak independence and heterogeneous distribution of $\{\hat{X}_1, \dots, \hat{X}_n\}$ by modifying proofs. This will accommodate weakly dependent functional data or the contaminated \hat{X}_i that are attained by borrowing information across individuals (e.g. Yao et al., 2005a), which is beyond our scope here and can be a topic of future research.

The contamination of the predictor X poses substantial challenge on the estimation of the manifold structures. For instance, the quality of the tagant space at x , denoted by $T_x\mathcal{M}$, crucially depend on a bona fide neighborhood around x , while the contaminated neighborhood $\hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)$ and the inaccessible true neighborhood $\mathcal{N}_{\mathcal{L}^2}(h_{pca}, x) = \{X_i : \|X_i - x\|_{\mathcal{L}^2} < h_{pca}\}$ might contain different observations. Fortunately we can show that they are not far apart in the sense of Proposition S.2 in the Supplementary Material. In practice, we suggest to choose $\max(h_{reg}, h_{pca}) < \min\{2/\tau, \text{inj}(\mathcal{M})\}/4$, where τ is the condition number of \mathcal{M} and $\text{inj}(\mathcal{M})$ is the injectivity radius of \mathcal{M} (Cheng and Wu, 2013), so that $\hat{\mathcal{N}}_{\mathcal{L}^2}(h_{pca}, x)$ provides a good approximation of the true neighborhood of x within the manifold. The following result concerns the estimation quality of the local manifold structures, where $\iota_*T_x\mathcal{M}$ represents the embedded tangent space at $\iota(x)$, with ι_* denoting the pushforward of the embedding ι .

THEOREM 2. *Under assumptions (B1) and (B3), we have*

- (a) \hat{d} is a consistent estimate of d when $\min\{k_1, k_2\} \rightarrow \infty$ and $\max\{k_1, k_2\}/n \rightarrow 0$.
- (b) Let $\varrho = 1/(d+2)$ if $\beta \geq 2/d$ and $\varrho = \beta/2$ otherwise, $h_{pca} \asymp n^{-\varrho}$. Then the eigenbasis $\{\hat{\varphi}_k\}_{k=1}^d$ derived from \hat{C}_x in (6) is close to an orthonormal basis $\{\phi_k\}_{k=1}^d$ of $T_x\mathcal{M}$: if $x \in \mathcal{M}$, for $k = 1, 2, \dots, d$,

$$\hat{\varphi}_k = \iota_*\phi_k + O_P(h_{pca}^{3/2})\mathbf{u}_k + O_P(h_{pca})\mathbf{u}_k^\perp, \quad (10)$$

where $\mathbf{u}_k \in \iota_* T_x \mathcal{M}$, $\mathbf{u}_k^\perp \perp \iota_* T_x \mathcal{M}$, and $\|\mathbf{u}_k\|_{\mathcal{L}^2} = \|\mathbf{u}_k^\perp\|_{\mathcal{L}^2} = 1$.

In light of Theorem 2(a), we shall from now on present the subsequent results by conditioning on the event $\hat{d} = d$, and the top-right panel of Figure 1 provides a geometric illustration of equation (10) for the case $d = 2$.

Now we begin to state the results on the estimated regression functional. Recall that $\hat{g}(x)$ in (7) is obtained by applying local linear smoother on the coordinates of contaminated predictors within the estimated tangent space at x . It is well known that local linear estimator does not suffer from boundary effects, i.e., the first order behavior of the estimator at the boundary is the same as in the interior (Fan, 1992). However, the contamination on predictor has different impact, and we shall address the interior and boundary cases separately. Denote $\mathcal{D} = \{(\hat{X}_1, Y_1), (\hat{X}_2, Y_2), \dots, (\hat{X}_n, Y_n)\}$ and $\mathcal{M}_h = \{x \in \mathcal{M} : \inf_{y \in \partial \mathcal{M}} \mathfrak{d}(x, y) \leq h\}$, where $\partial \mathcal{M}$ denotes the boundary of \mathcal{M} and $\mathfrak{d}(\cdot, \cdot)$ denotes the distance function on \mathcal{M} . For points sufficiently far away from the boundary of \mathcal{M} , we have the following result about the conditional MSE of the estimate $\hat{g}(x)$.

THEOREM 3. *Assume that (A1) and (B1)–(B3) hold. Let $x \in \mathcal{M} \setminus \mathcal{M}_{h_{reg}}$ and h_{pca} chosen as in Theorem 2(b). For any $\epsilon > 0$, if we choose $h_{reg} \asymp n^{-1/(d+4)}$ when $\beta > 3/(d+4)$, and $h_{reg} \asymp n^{-\beta/(3+\epsilon d)}$ when $\beta \leq 3/(d+4)$, then*

$$\mathbf{E} \left[\{\hat{g}(x) - g(x)\}^2 \mid \mathcal{D} \right] = O_P \left(n^{-\frac{4}{d+4}} + n^{-\frac{4\beta}{3+\epsilon}} \right). \quad (11)$$

We emphasize the following observations from this theorem. First, the convergence rate of $\hat{g}(x)$ is a polynomial of the sample size n depending on both the intrinsic dimension d and the *contamination level* defined as $\gamma = \beta^{-1}$. This is in contrast with traditional functional nonparametric regression methods that do not explore the intrinsic structure, which cannot reach a polynomial rate of convergence. Second, when contamination level $\gamma < \gamma_0 = (d+4)/3$, the intrinsic dimension dominates the convergence rate in (11), while when $\gamma \geq \gamma_0$, the contamination dominates. Thus the convergence rate exhibits a phase transition separated at the threshold level γ_0 . Intuitively, when the contamination is low, the manifold structure can be estimated reliably and hence determines the quality of the estimated regression. On the other hand, when the contamination passes the

threshold γ_0 , the manifold structure is buried by noise and cannot be well utilized. We illustrate this graphically in the bottom panels of Figure 1. Third, it is observed that the phase transition threshold γ_0 increases with the intrinsic dimension d that indicates the complexity of a manifold. This interesting finding suggests that, although estimating a complex manifold is more challenging (i.e., slower rate), such a manifold is more resistant to contamination.

Theorem 3 can be also interpreted by relating the sampling rate m and the sample size n . Recall that $m \geq n^\alpha$ and $\gamma = (2 + \nu^{-1})/\alpha$, where ν denotes the Hölder smoothness of the process X as in (A3). When the sampling rate is low, $\alpha \leq 3(2 + \nu^{-1})/(d + 4)$, i.e., $m \lesssim n^{3(2+\nu^{-1})/(d+4)}$, the contamination reflected by the second term in the right hand side (r.h.s.) of (11) dominates and is actually determined by m . Otherwise the first term prevails and involves only the sample size n and the intrinsic dimension prevails. In the literature of functional data analysis, ν is typically at least 2, i.e., continuously twice differentiable. For a moderate dimension such as $d = 6$, the contamination blurs the estimation of g when $m \lesssim n^{3/4}$, and becomes asymptotically negligible otherwise, where $a_n \lesssim b_n$ denotes $a_n/b_n \rightarrow 0$. Next theorem characterize the asymptotic behavior of \hat{g} at x close to close to the boundary of \mathcal{M} .

THEOREM 4. *Assume that (A1) and (B1)–(B3) hold. Let $x \in \mathcal{M}_{h_{reg}}$ and h_{pca} chosen as in Theorem 2. For any $\epsilon > 0$, if we choose $h_{reg} \asymp n^{-1/(d+4)}$ when $\beta > 4/(d+4)$, and $h_{reg} \asymp n^{-\beta/(4+\epsilon d)}$ when $\beta \leq 4/(d+4)$, then the conditional MSE satisfies*

$$\mathbf{E} \left[\{\hat{g}(x) - g(x)\}^2 \mid \mathcal{D} \right] = O_P \left(n^{-\frac{4}{d+4}} + n^{-\frac{4\beta}{4+\epsilon}} \right).$$

It is interesting to note that the effect of the intrinsic dimension on convergence is the same, regardless where \hat{g} is evaluated on the manifold. However, the effect of contamination behaves differently, due to the fact that the second order behavior of local linear estimator that depends on the location needs to be taken into account when there is contamination on X . We see that when contamination effect dominates, the convergence is slightly slower for boundary points than for interior points, and the phase transition occurs at $\gamma_0 = (d + 4)/4$. This is the price we pay for the boundary effect when predictors are contaminated, which is in contrast with the classical result on local linear estimator (Fan, 1993).

4. Simulation Study

To demonstrate the performance of the proposed manifold approach, we conduct simulations for three different manifold structures, namely, the three-dimensional rotation group $SO(3)$, the Klein bottle (Klein) and the mixture of two Gaussian densities (MixG). For all settings, a functional predictor X_i is observed at $m = 100$ equally spaced points T_1, T_2, \dots, T_m in the interval $[0, 1]$ with heteroscedastic measurement error $\epsilon_{ij} \sim N(0, \sigma_j^2)$, where σ_j is determined by the signal-to-noise ratio on $X(T_j)$ so that $\text{snrdb}_X = \text{Var}\{X(T_j)\}/\sigma_j^2 = 4$. The noise ε_i on response Y is a centred Gaussian variable with variance σ_ε^2 that is determined by the signal-to-noise ratio on Y so that $\text{snrdb}_Y = \text{Var}(Y)/\sigma_\varepsilon^2 = 2$. Detailed information of each setting is provided below.

- **SO(3):** $X_i(t) = \mu(t) + \sum_{k=1}^9 \xi_{ik} b_k(t)$, where $\mu(t) = t + \sin(t)$, $b_{2\ell-1}(t) = \cos\{(2\ell-1)\pi t/10\}/\sqrt{5}$, $b_{2\ell}(t) = \sin\{(2\ell-1)\pi t/10\}/\sqrt{5}$. To generate random variables ξ_{ik} , we define vector $\mathbf{r} = (r_1, r_2, r_3)$ and matrix

$$\mathbf{R}(\mathbf{r}, \theta) = (1 - \cos \theta) \mathbf{r} \mathbf{r}^T + \begin{pmatrix} \cos \theta & -r_3 \sin \theta & r_2 \sin \theta \\ r_3 \sin \theta & \cos \theta & -r_1 \sin \theta \\ -r_2 \sin \theta & r_1 \sin \theta & \cos \theta \end{pmatrix}.$$

Denote $\mathbf{e}_2 = (1, 0, 0)^T$ and similarly \mathbf{e}_3 , and we generate $(\xi_{i1}, \dots, \xi_{i9})^T = \text{vec}(\mathbf{Z}_i)$ with

$$\mathbf{Z}_i = \mathbf{R}(\mathbf{e}_3, u_i) \mathbf{R}(\mathbf{e}_2, v_i) \mathbf{R}(\mathbf{e}_3, w_i), \quad (12)$$

where (u_i, v_i) are i.i.d. random pairs uniformly distributed on the 2D sphere $S^2 = [0, 2\pi) \times [0, \pi]$, and w_i is i.i.d. uniformly distributed on the unit circle $S^1 = [0, 2\pi)$. Note that (12) is the Euler angles parameterization of $SO(3)$ (Stuelpnagel, 1964) that has an intrinsic dimension $d = 3$. The response is generated by $Y_i = 2 \sin(2(u_i + w_i)) \cos(4v_i) + 4 \exp\{-16(u_i + w_i - v_i - 2\pi)^2\} + \varepsilon_i$.

- **Klein:** $X_i(t) = \mu(t) + \sum_{k=1}^4 \xi_{ik} \phi_k(t)$ with μ and ϕ_k as in the $SO(3)$ setting. For random variables ξ_k , we use $\xi_{i1} = (2 \cos v_i + 1) \cos u_i$, $\xi_{i2} = (2 \cos v_i + 1) \sin u_i$, $\xi_{i3} = 2 \sin v_i \cos(u_i/2)$ and $\xi_{i4} = 2 \sin v_i \sin(u_i/2)$, where $u_i, v_i \stackrel{i.i.d.}{\sim} \text{Unif}(0, 2\pi)$. Here $(u, v) \mapsto (\xi_1, \xi_2, \xi_3, \xi_4)$ provides

a parametrization of Klein bottle with an intrinsic dimension $d = 2$. The response is generated by $Y_i = 7 \sin(4u_i) + 5 \cos^2(2v_i) + 6 \exp\{-32[(u_i - \pi)^2 + (v_i - \pi)^2]\} + \varepsilon_i$.

- **MixG**: X_i is a mixture of two Gaussian densities, i.e., $X_i(t) = \exp\{-(t - u_i)^2/2\}/\sqrt{2\pi} + \exp\{-(t - v_i)^2/2\}/\sqrt{2\pi}$ with $(v_1, v_2)^T$ uniformly sampled from a circle with diameter 0.5, similar to that used in Chen and Müller (2012). The response is generated by $Y_i = 2 \exp\{0.1(u_i - \pi)^2\} \cos u_i \sin u_i + \varepsilon_i$.

Note that, according to Gräf and Potts (2009), our sampling yields also a uniform sample in the $SO(3)$ setting, while the uniform sampling on the parameter space (u_i, v_i) results in non-uniform sampling on the manifold in the Klein setting. In order to account for at least 95% of variance of the contaminated data, we find empirically that more than 10 principal components are needed in both settings, i.e., the dimensions of the contaminated data are considerably larger than their intrinsic dimensions.

For each setting, two different sample sizes are considered, $n = 500$ and $n = 1000$. For evaluation, we generate independent test data of size 5000, and compute the square-root of mean square error (rMSE) using the test data. For comparison, we compute the rMSE for various functional non-parametric regression methods described in Ferraty and Vieu (2006): functional Nadaraya-Waston estimator (FNW), functional conditional expectation (FCE), functional mode (FMO), functional conditional median (FCM) and the multi-method (MUL) that averages estimates from FCE, FMO and FCM. Functional linear regression (FLR) is also included to illustrate the impact of nonlinear relationship not captured by FLR. The tuning parameters in these methods, such as the number of principal components for FLR and the bandwidth for FNW, FCE, FMO and FCM, are selected by 10-fold cross validation. We repeat each study 100 times independently, and the results are presented in Table 4, based on which we conclude that the proposed method enjoys favorable numerical performance in all simulation settings. We also see that, for a larger sample, the reduction in rMSE is more prominent for the proposed method than for the other methods. This may provide some numerical evidence that the proposed estimator has indeed a faster convergence compared to its counterparts (Mas, 2012), owing to exploiting the underlying manifold structures.

Table 1. Shown are the Monte Carlo averages of square-root mean square error (rMSE) and its standard error in parenthesis based on 100 independent simulation runs, for different settings and methods described in Section 4.

	$SO(3)$		Klein Bottle		MixG	
	$n = 500$	$n = 1000$	$n = 500$	$n = 1000$	$n = 500$	$n = 1000$
FLR	2.68(.021)	2.62(.023)	5.30(.038)	5.28(.038)	1.04(.007)	1.03(.007)
FNW	2.61(.023)	2.59(.021)	4.85(.054)	4.79(.042)	.282(.013)	.274(.009)
FCE	2.59(.032)	2.52(.028)	4.84(.073)	4.63(.055)	.349(.016)	.341(.013)
FMO	3.43(.130)	3.33(.098)	6.61(.285)	6.44(.265)	.564(.034)	.528(.026)
FCM	2.69(.044)	2.62(.027)	5.30(.101)	5.08(.063)	.419(.019)	.382(.012)
MUL	2.73(.043)	2.64(.031)	5.19(.112)	5.02(.076)	.380(.017)	.351(.013)
Proposed	2.15(.061)	1.83(.038)	2.91(.143)	2.34(.062)	.120(.015)	.103(.011)

5. Real Data Examples

We apply the proposed method to analyze two real datasets. For the purpose of evaluation, we train our method on 75% of each dataset and reserve the other 25% as test data. The rMSE is computed on the held-out test data. For comparison, we also compute rMSE for FLR, FNW, FCE, FMO and FCM as described in Section 4. We repeat this 100 times based on random partitions of the datasets, and present the Monte Carlo averages of rMSE together with their standard errors in Table 2.

The first application is to predict fat content of a piece of meat based on a spectrometric curve of spectra of absorbances for the meat using the Tecator dataset with 215 meat samples (Ferraty and Vieu, 2006). For each sample, The spectrometric curve for a piece of finely chopped pure meat was measured at 100 different wavelengths from 850 to 1050nm. Along with spectrometric curves, the fat content for each piece of meat was recorded. Comparing to the analytic chemistry required for measuring the fat content, obtaining a spectrometric curve is less time and cost consuming. As in Ferraty and Vieu (2006), we predict the fat content based on the first derivative curves approximated by the difference quotient between measurements at adjacent wavelengths, shown in the left panel of Figure 2. It is seen that there are some striking patterns around the middle wavelengths. The proposed method is able to capture these patterns by a low-dimensional manifold structure and yields more efficient estimates of fat content. For example, the FLR model uses 15.7 principal components on average with standard error 1.07, while the intrinsic dimension

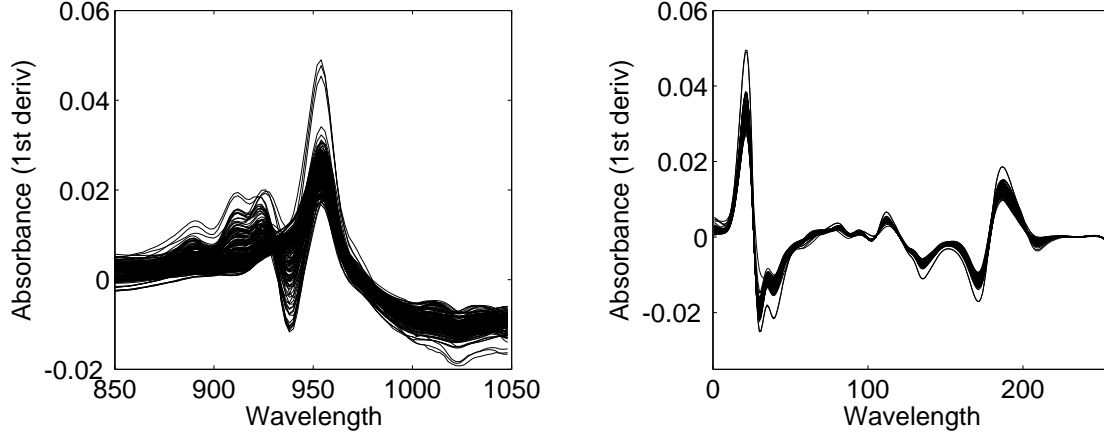


Fig. 2. Left: first derivative curves of the spectra of absorbance for finely chopped 215 pure meat samples. Right: first derivative curves of infrared spectra for 123 wine samples.

estimated by the proposed method is 5.05 with a standard error 0.62. From Table 2, the proposed method predicts the fat content more accurately than the other methods by a significant margin.

The second data example concerns estimating alcohol level based on infrared spectrum of wine, provided by Professor Marc Meurens, Université Catholique de Louvain. The data contains a training set of 94 samples and a test set of 30 samples, which are combined to give a total dataset of size 123 after removing the 84th sample due to outliers. Each sample includes the mean infrared spectrum of a wine observed at 256 points and the corresponding alcohol level, and the first derivative curves approximated by difference quotient that our analysis is based on are shown in the right panel of Figure 2. The average of estimated intrinsic dimensions is 1.72 with standard error 0.26. By contrast, the average number of principal components for FLR is 3.080 with standard error 0.339. From Table 2, our method enjoys the most accurate prediction, followed by the FLR, while all other functional nonparametric methods deteriorate considerably.

Acknowledgements

This research is partially supported by Natural Science and Engineering Research Council of Canada.

Table 2. Shown are the Monte Carlo averages of square-root mean square error (rmSE) and its standard error based on 100 random partitions, for different methods on the meat spectrometric data and wine spectrometric data, where the results for wine spectrometric data is multiplied by 10 for visualization.

	FLR	FNW	FCE	FMO	FCM	MUL	Proposed
Meat	2.56(.433)	2.42(.334)	1.97(.354)	2.66(.459)	2.82(.454)	2.31(.354)	1.06(.344)
Wine	1.36(.281)	5.14(1.97)	5.14(2.38)	7.82(3.03)	7.86(3.36)	6.65(2.96)	1.17(.203)

Appendix A: Proofs of Main Theorems

We provide below the proofs of Theorem 1–3 as well as Corollary 1, while the proof of Theorem 4 using similar techniques is deferred to the Supplementary Material. In order to reduce notational burden, $\mathcal{L}^2(D)$ is simplified by \mathcal{L}^2 , and we shall use $\|\cdot\|$ to denote the norm $\|\cdot\|_{\mathcal{L}^2}$ when no confusion arises.

PROOF OF THEOREM 1 AND COROLLARY 1. In order to reduce notations, let $h = h_0$. Denoting $\Delta = \delta 1_{|S_0 S_2 - S_1^2| < \delta}$ with $\delta = m^{-2}$, according to (4), we have

$$\hat{X}(t) - X(t) = \frac{S_2(R_0 - S_0 X)}{S_0 S_2 - S_1^2 + \Delta} - \frac{S_1(R_1 - S_1 X)}{S_0 S_2 - S_1^2 + \Delta} - \frac{\Delta X}{S_0 S_2 - S_1^2 + \Delta} \equiv I_1 + I_2 + I_3.$$

Therefore,

$$\|\hat{X} - X\|^p \leq c_p(\|I_1\|^p + \|I_2\|^p + \|I_3\|^p) \quad (13)$$

for some constant c_p depending on p only.

For I_1 , we have

$$\begin{aligned} \|I_1\|^p &= \left[\int_D \left\{ \frac{S_2(R_0 - S_0 X)}{S_0 S_2 - S_1^2 + \Delta} \right\}^2 dt \right]^{p/2} \leq \left[\int_D \{S_2(R_0 - S_0 X)\}^4 dt \int_D \left(\frac{1}{S_0 S_2 - S_1^2 + \Delta} \right)^4 dt \right]^{p/4} \\ &\leq \left\{ \int_D S_2^8 dt \int_D (R_0 - S_0 X)^8 dt \right\}^{p/8} \left\{ \int_D \left(\frac{1}{S_0 S_2 - S_1^2 + \Delta} \right)^4 dt \right\}^{p/4}. \end{aligned}$$

This also shows that, for $p \geq 2$,

$$\begin{aligned}
& \mathbf{E}(\|I_1\|^p \mid X) \\
& \leq \left(\mathbf{E} \left\{ \left[\int_D S_2^8 dt \int_D (R_0 - S_0 X)^8 dt \right]^{p/4} \mid X \right\} \right)^{1/2} \left(\mathbf{E} \left\{ \left[\int_D \left(\frac{1}{S_0 S_2 - S_1^2 + \Delta} \right)^4 dt \right]^{p/2} \mid X \right\} \right)^{1/2} \\
& \leq \left(\mathbf{E} \left[\int_D S_2^{4p} dt \right] \mathbf{E} \left[\int_D (R_0 - S_0 X)^{4p} dt \mid X \right] \right)^{1/4} \left(\mathbf{E} \left[\int_D \left\{ \frac{1}{S_0 S_2 - S_1^2 + \Delta} \right\}^{2p} dt \right] \right)^{1/2} \\
& = \left\{ \int_D \mathbf{E}(S_2^{4p}) dt \right\}^{1/4} \left[\int_D \mathbf{E}\{(R_0 - S_0 X)^{4p} \mid X\} dt \right]^{1/4} \left[\int_D \mathbf{E} \left\{ \left(\frac{1}{S_0 S_2 - S_1^2 + \Delta} \right)^{2p} \right\} dt \right]^{1/2}.
\end{aligned} \tag{14}$$

Let $E_{0,X} = \mathbf{E}(R_0 - S_0 X \mid X)$ and ℓ be the largest integer strictly less than ν . By Taylor expansion,

$$\begin{aligned}
E_{0,X} &= \mathbf{E} \left[\frac{1}{mh} \sum_{j=1}^m K \left(\frac{T_j - t}{h} \right) \{X(T_j) + \zeta_j - X(t)\} \mid X \right] \\
&= \frac{1}{mh} \sum_{j=1}^m \mathbf{E} \left[K \left(\frac{T_j - t}{h} \right) \left\{ \frac{X^{(\ell)}(t + \tau_j(T_j - t)) - X^{(\ell)}(t)}{\ell!} (T_j - t)^\ell \right\} \mid X \right],
\end{aligned}$$

where $\tau_j \in [0, 1]$. Hence,

$$\begin{aligned}
|E_{0,X}| &\leq \frac{1}{mh} \sum_{j=1}^m \mathbf{E} \left\{ K \left(\frac{T_j - t}{h} \right) \left| \frac{X^{(\ell)}(t + \tau_j(T_j - t)) - X^{(\ell)}(t)}{\ell!} (T_j - t)^\ell \right| \mid X \right\}, \\
&\leq \frac{1}{h\ell!} L_X \mathbf{E} \left\{ K \left(\frac{T - t}{h} \right) |T - t|^\nu \right\} \leq \frac{L_X C_{T,2}}{\ell!} h^\nu u_\nu,
\end{aligned} \tag{15}$$

where $u_\nu = \int_{-1}^1 K(s) |s|^\nu ds$. Let $\sigma_{r,X} = \mathbf{E} \left([h^{-1} K \{(T_j - t)/h\} \{X(T_j) + \zeta_j - X(t)\} - E_{0,X}]^r \mid X \right)$.

Then, for $r \geq 2$,

$$\begin{aligned}
\sigma_{r,X} &= \mathbf{E} \left(\left[\frac{1}{h} K \left(\frac{T_j - t}{h} \right) \{X(T_j) + \zeta_j - X(t)\} - E_{0,X} \right]^r \mid X \right) \\
&\leq 3^r \mathbf{E} \left[\left\{ \frac{1}{h} K \left(\frac{T_j - t}{h} \right) |X(T_j) - X(t)| \right\}^r \mid X \right] + 3^r \mathbf{E} \left[\left\{ \frac{1}{h} K \left(\frac{T_j - t}{h} \right) |\zeta_j| \right\}^r \mid X \right] + 3^r |E_{0,X}|^r \\
&\leq 2 \cdot 3^r \left\{ \sup_t |X(t)|^r \right\} \mathbf{E} \left[\left\{ \frac{1}{h} K \left(\frac{T_j - t}{h} \right) \right\}^r \right] + 3^r \mathbf{E} \left[\left\{ \frac{1}{h} K \left(\frac{T_j - t}{h} \right) \right\}^r |\zeta_j|^r \right] + 3^r |E_{0,X}|^r \\
&\leq 2 \cdot 3^r \left\{ \sup_t |X(t)|^r \right\} h^{1-r} C_{T,2}^r + 3^r h^{1-r} C_{T,2}^r \mathbf{E} |\zeta|^r + 3^r L_X^r C_{T,2}^r h^{r\nu} u_\nu^r.
\end{aligned} \tag{16}$$

With (15) and (16), by Lemma S.4, conditioning on X , we have

$$\mathbf{E} \{ (R_0 - S_0 X - E_{0,X})^{4p} \mid X \} \leq c_1(p) C_{T,2}^{4p} \{ \sup_t |X(t)|^{4p} + L_X^{4p} u_\nu^{4p} \} m^{-2p} h^{-2p},$$

where $c_j(p)$ denote a constant depending on p only for any j . This implies that

$$\begin{aligned}
\mathbf{E} \{ (R_0 - S_0 X)^{4p} \mid X \} &\leq 2^{4p} \mathbf{E} \{ (R_0 - S_0 X - E_{0,X})^{4p} \mid X \} + 2^{4p} \mathbf{E} \{ (E_{0,X})^{4p} \mid X \} \\
&\leq 2^{4p} c_1(p) C_{T,2}^{4p} \{ \sup_t |X(t)|^{4p} + L_X^{4p} u_\nu^{4p} \} m^{-2p} h^{-2p} + (2C_{T,2} u_\nu)^{4p} h^{4p\nu} L_X^{4p}.
\end{aligned} \tag{17}$$

By a similar argument, we can show that $\mathbf{E}(S_2 - \mathbf{E}S_2)^{4p} \leq c_2(p) m^{-2p} h^{-2p}$. Also, it is easy to check that $C_{T,1} u_2 \leq \mathbf{E}S_2 \leq C_{T,2} u_2$ with u_q denoting $\int_{-1}^1 K(u) |u|^q du$ and hence

$$\mathbf{E}(S_2^{4p}) \leq 2^{4p} \mathbf{E}(S_2 - \mathbf{E}S_2)^{4p} + 2^{4p} |\mathbf{E}S_2|^{4p} \leq C_{T,2}^{4p} u_2^{4p} + c_2(p) m^{-2p} h^{-2p} = O(1). \tag{18}$$

The same argument leads to $\mathbf{E}\{S_0 S_2 - S_1^2 - \mathbf{E}(S_0 S_2 - S_1^2)\}^{2p} \leq c_3(p) m^{-p} h^{-p}$. Note that $\inf_t \mathbf{E}(S_0 S_2 - S_1^2) > 0$ so that $\{\mathbf{E}(S_0 S_2 - S_1^2)\}^{-1} = O(1)$. By Lemma S.5, this also implies that

$$\int_D \mathbf{E} \left\{ \left(\frac{1}{S_0 S_2 - S_1^2 + \Delta} \right)^{2p} \right\} dt = O(1) + O(m^{-p} h^{-p} + m^{-4p}) = O(1). \tag{19}$$

Putting (14), (17), (18) and (19) together, we conclude that

$$\mathbf{E}(\|I_1\|^p \mid X) = c_4(p) \left[\left\{ \sup_t |X(t)|^p + L_X^p \right\} m^{-p/2} h^{-p/2} + h^{p\nu} L_X^p \right]. \tag{20}$$

The same rate for I_2 can be obtained in a similar fashion. For I_3 , we have

$$\|I_3\|^p = \left\{ \int_D \left(\frac{\Delta X}{S_0 S_2 - S_1^2 + \Delta} \right)^2 dt \right\}^{p/2} \leq \Delta^p \sup_t |X(t)|^p \left\{ \int_D \left(\frac{1}{S_0 S_2 - S_1^2 + \Delta} \right)^2 dt \right\}^{p/2}.$$

Therefore, with (19),

$$\mathbf{E}(\|I_3\|^p \mid X) \leq \Delta^p \sup_t |X(t)|^p \int_D \mathbf{E} \left\{ \left(\frac{1}{S_0 S_2 - S_1^2 + \Delta} \right)^{2p} \right\} dt \leq O(m^{-2p}) \sup_t |X(t)|^p. \quad (21)$$

Now, by (20) and (21), observing that m^{-2p} is asymptotically dominated by $m^{-p/2} h^{-p/2}$, with (13) we conclude that

$$\mathbf{E}(\|\hat{X} - X\|^p \mid X) = O(m^{-p/2} h^{-p/2}) \{ \sup_t |X(t)|^p + L_X^p \} + O(h^{p\nu}) L_X^p. \quad (22)$$

Then the statement (8) follows by $p \geq 1$. When $h_0 \asymp m^{-\frac{1}{2\nu+1}}$, $m^{-1/2} h^{-1/2} \asymp h^\nu \asymp m^{-\frac{\nu}{2\nu+1}}$, and the statement (9) follows. Corollary 1 is also an immediate consequence of (22). \square

PROOF OF THEOREM 2. (a) Without loss of generality, assume $x = 0$. Let $\tilde{G}_j = \hat{G}_j + \Delta$ and $\tilde{G}_{(1)}, \tilde{G}_{(2)}, \dots, \tilde{G}_{(k)}$ be the associated order statistics of $\tilde{G}_1, \tilde{G}_2, \dots, \tilde{G}_k$. Then,

$$\begin{aligned} & \left| \frac{1}{k-1} \sum_{j=1}^{k-1} \log \frac{\hat{G}_{(k)} + \Delta}{\hat{G}_{(j)} + \Delta} - \frac{1}{k-1} \sum_{j=1}^{k-1} \log \frac{G_{(k)}}{G_{(j)}} \right| \\ & \leq \left| \log \tilde{G}_{(k)} - \log G_{(k)} \right| + \left| \frac{1}{k-1} \sum_{j=1}^k \left(\log \tilde{G}_{(j)} - \log G_{(j)} \right) \right| \equiv I_1 + I_2. \end{aligned} \quad (23)$$

For I_1 , let q and q be the indices such that $\tilde{G}_{(k)} = \hat{G}_q$ and $G_p = G_{(k)}$, respectively. For the case $q = p$, we have $|\tilde{G}_{(k)} - G_{(k)}| = |\tilde{G}_p - G_p| \leq \left| \|\hat{X}_p\| - \|X_p\| \right| + \Delta \leq \|\hat{X}_p - X_p\| + \Delta$ by reverse triangle inequality. When $q \neq p$, it is seen that $\tilde{G}_p < \tilde{G}_{(k)} = \tilde{G}_q$ and $G_q < G_p = G_{(k)}$. If $\tilde{G}_{(k)} > G_{(k)}$, then $|\tilde{G}_{(k)} - G_{(k)}| \leq |\tilde{G}_{(k)} - G_q| = |\tilde{G}_q - G_q| \leq \max_{1 \leq j \leq k} \{\|\hat{X}_j - X_j\|\} + \Delta$. Otherwise, $|\tilde{G}_{(k)} - G_{(k)}| \leq |\tilde{G}_p - G_p| \leq \max_{1 \leq j \leq k} \{\|\hat{X}_j - X_j\|\} + \Delta$. Now, $\Pr(\forall 1 \leq j \leq k : \|\hat{X}_j - X_j\| > \epsilon) \leq$

$\sum_{j=1}^k \Pr \left(\|\hat{X}_j - X_j\| > \epsilon \right) \leq k \mathbf{E} \|\hat{X}_j - X_j\|^r \epsilon^{-r} = O(kn^{-r\beta}) = o(1)$ for a sufficiently large constant r . Therefore, $|\tilde{G}_{(k)} - G_{(k)}|$ converges to zero in probability, or $\tilde{G}_{(k)}$ converges to $G_{(k)}$ in probability. By Slutsky's lemma, $\log \tilde{G}_{(k)}$ converges to $\log G_{(k)}$ in probability and hence $I_1 = o_P(1)$.

For I_2 , we first observe that

$$I_2 = \left| \frac{1}{k-1} \sum_{j=1}^k \left(\log \tilde{G}_{(j)} - \log G_{(j)} \right) \right| = \left| \frac{1}{k-1} \sum_{j=1}^k \left(\log \tilde{G}_j - \log G_j \right) \right|.$$

By Markov's inequality, for any fixed $\epsilon > 0$,

$$\Pr(I_{21} > \epsilon) \leq \frac{\mathbf{E} I_{21}}{\epsilon} \leq \frac{k \mathbf{E} |\log \hat{G} - \log G|}{(k-1)\epsilon} = o(1),$$

where the last equality is obtained by Lemma S.6. We then deduce that $I_2 = o_P(1)$. Together with $I_1 = o_P(1)$ and (23), this implies that

$$\left| \frac{1}{k-1} \sum_{j=1}^{k-1} \log \frac{\hat{G}_{(k)} + \Delta}{\hat{G}_{(j)} + \Delta} - \frac{1}{k-1} \sum_{j=1}^{k-1} \log \frac{G_{(k)}}{G_{(j)}} \right| \rightarrow 0 \quad \text{in probability.}$$

Now we apply the argument in Levina and Bickel (2004) to conclude that \hat{d} is a consistent estimator.

(b) Let $h = h_{pca}$, and $\{\tilde{\phi}_k\}_{k=1}^d$ be a orthonormal basis system for $\iota_* T_x \mathcal{M}$ and $\{\psi_k\}_{k=1}^\infty$ be an orthonormal basis of \mathcal{L}^2 . Assume that \mathcal{M} is properly rotated and translated so that $\psi_k = \tilde{\phi}_k$ for $k = 1, 2, \dots, d$, and $x = 0 \in \mathcal{L}^2$. The sample covariance operator based on observations in $\hat{\mathcal{N}}_{\mathcal{L}^2}(h, x)$ is denoted by $\hat{\mathcal{C}}_x$ as in (6). It is seen that $\hat{\mathcal{C}}_x = n^{-1} \sum_{i=1}^n (\hat{X}_i - \hat{\mu}_x)(\hat{X}_i - \hat{\mu}_x) Z_i$, where $Z_i = 1_{\{\hat{X}_i \in \mathbb{B}_h^{\mathcal{L}^2}(x)\}}$ and $\hat{\mu}_x = n^{-1} \sum_{i=1}^n \hat{X}_i Z_i$. Let $\mathcal{H}_1 = \text{span}\{\psi_k : k = 1, 2, \dots, d\}$ and \mathcal{H}_2 be the complementary subspace of \mathcal{H}_1 in \mathcal{L}^2 , so that $\mathcal{L}^2 = \mathcal{H}_1 \oplus \mathcal{H}_2$. Let $\mathcal{P}_j : \mathcal{L}^2 \rightarrow \mathcal{H}_j$ be projection operators, and we define operator $\mathcal{A} = \mathcal{P}_1 \hat{\mathcal{C}}_x \mathcal{P}_1$, $\mathcal{B} = \mathcal{P}_2 \hat{\mathcal{C}}_x \mathcal{P}_2$, $\mathcal{D}_{12} = \mathcal{P}_1 \hat{\mathcal{C}}_x \mathcal{P}_2$ and $\mathcal{D}_{21} = \mathcal{P}_2 \hat{\mathcal{C}}_x \mathcal{P}_1$. Then $\hat{\mathcal{C}}_x = \mathcal{A} + \mathcal{B} + \mathcal{D}_{12} + \mathcal{D}_{21}$. Note that $\mathcal{D}_{12} + \mathcal{D}_{21}$ is self-adjoint. Therefore, if $y = \sum_{k=1}^\infty a_k \psi_k \in \mathcal{L}^2$, then

$$\begin{aligned}
\|\mathcal{D}_{12} + \mathcal{D}_{21}\|_{op} &= \sup_{\|y\|=1} \langle (\mathcal{D}_{12} + \mathcal{D}_{21})y, y \rangle = \sup_{\|y\|=1} \left(\langle \mathcal{P}_1 \hat{\mathcal{C}}_x \mathcal{P}_2 y, y \rangle + \langle \mathcal{P}_2 \hat{\mathcal{C}}_x \mathcal{P}_1 y, y \rangle \right) \\
&= \sup_{\|y\|=1} \left(\langle \hat{\mathcal{C}}_x \mathcal{P}_2 y, \mathcal{P}_1 y \rangle + \langle \hat{\mathcal{C}}_x \mathcal{P}_1 y, \mathcal{P}_2 y \rangle \right) \\
&= 2 \sup_{\|y\|=1} \left(\sum_{k=d+1}^{\infty} \sum_{j=1}^d a_j a_k \langle \hat{\mathcal{C}}_x \psi_j, \psi_k \rangle \right) \leq 2 \sup_{\|y\|=1} \left(\sum_{k=d+1}^{\infty} \sum_{j=1}^d |a_j a_k| \cdot \left| \langle \hat{\mathcal{C}}_x \psi_j, \psi_k \rangle \right| \right) \\
&\leq 2 \sup_{j \leq d} \sup_{k \geq d+1} \left| \langle \hat{\mathcal{C}}_x \psi_j, \psi_k \rangle \right| \sup_{\|y\|=1} \left(\sum_{k=d+1}^{\infty} \sum_{j=1}^d |a_j a_k| \right) \\
&\leq \sup_{j \leq d} \sup_{k \geq d+1} \left| \langle \hat{\mathcal{C}}_x \psi_j, \psi_k \rangle \right| \sup_{\|y\|=1} \left\{ \sum_{k=d+1}^{\infty} \sum_{j=1}^d (a_j^2 + a_k^2) \right\} \leq 2 \sup_{j \leq d} \sup_{k \geq d+1} \left| \langle \hat{\mathcal{C}}_x \psi_j, \psi_k \rangle \right|.
\end{aligned}$$

From Lemma S.8, $\|\mathcal{D}_{12} + \mathcal{D}_{21}\|_{op} = O_P(h^{d+3} + n^{-1/2}h^{d/2+3} + n^{-\beta}h^{d+1})$. Similarly, we have $\|\mathcal{B}\|_{op} = O_P(h^{d+4} + n^{-1/2}h^{d/2+4} + n^{-\beta}h^{d+1})$, and $\mathcal{A} = \pi_{d-1}f(x)d^{-1}h^{d+2}\mathbf{I}_d + O_P(n^{-1/2}h^{d/2+2} + n^{-\beta}h^{d+1})$, where π_{d-1} is the volume of $d-1$ dimensional unit sphere, and \mathbf{I}_d is the identity operator on \mathcal{H}_1 .

By assumption on ϱ , we have $\varrho < \min\{1/d, \beta\}$. Then h^{d+2} is the dominant term. Let $a_n = n^{-1/2}h^{-d/2}$ and $b_n = n^{-\beta}h^{-1}$, we have

$$\hat{\mathcal{C}}_x = \pi_{d-1}f(x)d^{-1}h^{d+2}\{\mathbf{I}_d + O_P(a_n + b_n)\tilde{\mathcal{A}} + O_P(h^2 + b_n)\tilde{\mathcal{B}} + O_P(h + b_n)(\tilde{\mathcal{D}}_{12} + \tilde{\mathcal{D}}_{21})\}$$

where $\tilde{\mathcal{A}}$, $\tilde{\mathcal{B}}$, $\tilde{\mathcal{D}}_{12}$ and $\tilde{\mathcal{D}}_{21}$ are all with operator norm equal to one, and $\tilde{\mathcal{D}}_{12}$ is the adjoint of $\tilde{\mathcal{D}}_{21}$. With the choice of ϱ , we have

$$\hat{\mathcal{C}}_x = \pi_{d-1}f(x)d^{-1}h^{d+2}\left\{\mathbf{I}_d + O_P(\sqrt{h})\tilde{\mathcal{A}} + O_P(h)\tilde{\mathcal{B}} + O_P(h)(\tilde{\mathcal{D}}_{12} + \tilde{\mathcal{D}}_{21})\right\}.$$

The same perturbation argument done in Singer and Wu (2012) leads to the desired result. \square

PROOF OF THEOREM 3. The proof is analogous to that of Theorem 4.2 of Cheng and Wu (2013), except that we need to handle the extra issues caused by noise on X . For clarity, we give a

self-contained proof with emphasis on the extra issues. To reduce notions, let $h = h_{reg}$ and fix $x \in \mathcal{M}$. Let $\{\hat{\varphi}_k\}_{k=1}^d$ be the orthonormal set determined by local FPCA and $\{\phi_k\}_{k=1}^d$ the associated orthonormal basis of $T_x\mathcal{M}$. Let $\{\psi_k\}_{k=1}^\infty$ be an orthonormal basis of \mathcal{L}^2 . Assume ι is properly rotated and translated so that $\iota(x) = 0 \in \mathcal{L}^2$ and $\psi_k = \iota_*\phi_k$ for $k = 1, 2, \dots, d$. Let $\mathbf{g} = (g(X_1), g(X_2), \dots, g(X_n))^T$. Then we have

$$\mathbf{E}\{\hat{g}(x) \mid \mathcal{D}\} = \mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \mathbf{g}.$$

Take $z = \exp_x(t\theta)$, where $t = O(h)$, $\|\theta\|_{\mathcal{L}^2} = 1$ and \exp_x denotes the exponential map at x . By Theorem 2, we have $\langle \iota_*\theta, \hat{\varphi}_k \rangle = \langle \iota_*\theta, \psi_k \rangle + O_P(h_{pca}^{3/2})$ and $\langle \Pi_x(\theta, \theta), \hat{\varphi}_k \rangle = O_P(h_{pca})$. By Lemma A.2.2. of Cheng and Wu (2013), we have

$$t\iota_*\theta = \iota(y) - t^2\Pi_x(\theta, \theta)/2 + O(t^3). \quad (24)$$

Therefore, for $k = 1, 2, \dots, d$,

$$\begin{aligned} \langle t\iota_*\theta, \psi_k \rangle &= \langle t\iota_*\theta, \hat{\varphi}_k - O_P(h_{pca}^{3/2})\mathbf{u}_k \rangle = \langle \iota(z), \hat{\varphi}_k \rangle - t^2 \langle \Pi_x(\theta, \theta), \hat{\varphi}_k \rangle / 2 + O_P(hh_{pca}^{3/2} + h^2h_{pca}) \\ &= \langle \iota(z), \hat{\varphi}_k \rangle + O_P(hh_{pca}^{3/2} + h^2h_{pca}). \end{aligned}$$

Since ι is an embedding, we have $\theta = \sum_{k=1}^d \langle \iota_*\theta, \psi_k \rangle \phi_k$. Let $\mathbf{z} = (\langle \iota(z), \hat{\varphi}_1 \rangle, \langle \iota(z), \hat{\varphi}_2 \rangle, \dots, \langle \iota(z), \hat{\varphi}_d \rangle)^T$. By (24), it is easy to see that

$$\begin{aligned} g(x) - g(z) &= t\theta \nabla g(x) + \text{Hess } g(z)(\theta, \theta)t^2/2 + O_P(t^3) \\ &= \sum_{k=1}^d \langle t\iota_*\theta, \psi_k \rangle \nabla_{\phi_k} g(z) + \frac{1}{2} \sum_{j,k=1}^d \langle t\iota_*\theta, \psi_j \rangle \langle t\iota_*\theta, \psi_k \rangle \text{Hess } g(z)(\phi_j, \phi_k) + O_P(h^3) \\ &= \mathbf{z}^T \nabla g(x) + \frac{1}{2} \mathbf{z}^T \text{Hess } g(x) \mathbf{z} + O_P(h^3 + hh_{pca}^{3/2} + h^2h_{pca}) \\ &= \mathbf{z}^T \nabla g(x) + \frac{1}{2} \mathbf{z}^T \text{Hess } g(x) \mathbf{z} + O_P(h^{5/2}), \end{aligned}$$

where the last inequality is due to $h \geq h_{pca}$ implied by our choice of h and h_{pca} .

Due to smoothness of g , compactness of \mathcal{M} and the compact support of K , we have

$$\mathbf{g} = \mathbf{X} \begin{bmatrix} g(x) \\ \nabla g(x) \end{bmatrix} + \frac{\mathbf{H}}{2} + O_P(h^{5/2}),$$

where $\mathbf{H} = [\mathbf{x}_1^T \text{Hess } g(x) \mathbf{x}_1, \mathbf{x}_2^T \text{Hess } g(x) \mathbf{x}_2, \dots, \mathbf{x}_n^T \text{Hess } g(x) \mathbf{x}_n]^T$. Then the conditional bias is

$$\begin{aligned} \mathbf{E}\{\hat{g}(x) - g(x) \mid \mathcal{X}\} &= \mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \mathbf{g} - g(x) \\ &= \mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \left\{ \mathbf{X} \begin{bmatrix} g(x) \\ \nabla g(x) \end{bmatrix} + \frac{1}{2} \mathbf{H} + O_P(h^{5/2}) \right\} - g(x) \\ &= \mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \left\{ \mathbf{X} \begin{bmatrix} g(x) \\ \nabla g(x) \end{bmatrix} \right\} - g(x) + \mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \left\{ \frac{1}{2} \mathbf{H} + O_P(h^{5/2}) \right\} \\ &= \mathbf{e}_1^T \left(\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}} \right)^{-1} \frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} (\mathbf{X} - \hat{\mathbf{X}}) \begin{bmatrix} g(x) \\ \nabla g(x) \end{bmatrix} \end{aligned} \quad (25)$$

$$+ \mathbf{e}_1^T \left(\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}} \right)^{-1} \frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \left\{ \frac{1}{2} \mathbf{H} + O_P(h^{5/2}) \right\}. \quad (26)$$

Now we analyze the term in (25). Let $Z = 1_{\hat{X} \in \mathbb{B}_h^2(x)}$. By Lemma S.7, $\mathbf{E}Z \asymp h^d$. Then, by Hölder's inequality, for any fixed $\epsilon > 0$, we choose a constant $q > 1$ and a sufficiently large $p > 0$ so that $1/q + 1/p = 1$ and

$$\mathbf{E}Z \|\hat{X} - X\| = (\mathbf{E}Z)^{1/q} (\mathbf{E}\|\hat{X} - X\|^p)^{1/p} = O(h^{d-\epsilon d} n^{-\beta}).$$

Therefore,

$$\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} (\mathbf{X} - \hat{\mathbf{X}}) \begin{bmatrix} g(x) \\ \nabla g(x) \end{bmatrix} = \begin{bmatrix} \frac{1}{n} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|) (\mathbf{x}_i - \hat{\mathbf{x}}_i)^T \nabla g(x) \\ \frac{1}{n} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|) (\mathbf{x}_i - \hat{\mathbf{x}}_i)^T \nabla g(x) \hat{\mathbf{x}}_i \end{bmatrix} = O_P(h^{-1-\epsilon d} n^{-\beta}), \quad (27)$$

since

$$\begin{aligned} \left| \frac{1}{n} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|)(\mathbf{x}_i - \hat{\mathbf{x}}_i)^T \nabla g(x) \right| &\leq \frac{1}{n} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|) \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_{\mathbb{R}^d} \|\nabla g(x)\| \\ &\leq \{\sup_v |K(v)|\} \|\nabla g(x)\| \left(\frac{1}{n} \sum_{i=1}^n Z_i \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_{\mathbb{R}^d} \right) = O_P(h^{-1-\epsilon d} n^{-\beta}), \end{aligned}$$

and similarly, $n^{-1} \sum_{i=1}^n K_h(\|\hat{X}_i - x\|)(\mathbf{x}_i - \hat{\mathbf{x}}_i)^T \nabla g(x) \hat{\mathbf{x}}_i = O_P(h^{-1-\epsilon d} n^{-\beta}) \mathbf{1}_{d \times 1}$.

For $\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}}$, a direct calculation shows that

$$\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}} = \begin{bmatrix} n^{-1} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|) & n^{-1} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|) \hat{\mathbf{x}}_i^T \\ n^{-1} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|) \hat{\mathbf{x}}_i & n^{-1} \sum_{i=1}^n \hat{\mathbf{x}}_i^T K_h(\|\hat{X}_i - \iota(x)\|) \hat{\mathbf{x}}_i \end{bmatrix}.$$

It is easy to check that

$$n^{-1} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|) = n^{-1} \sum_{i=1}^n K_h(\|X_i - \iota(x)\|) + O_P(h^{-1-\epsilon d} n^{-\beta}),$$

and note that the choice of h ensures that $h^{1+\epsilon d} \gg n^{-\beta}$. Similar calculation shows that

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n K_h(\|\hat{X}_i - \iota(x)\|) \hat{\mathbf{x}}_i^T &= \frac{1}{n} \sum_{i=1}^n K_h(\|X_i - \iota(x)\|) \mathbf{x}_i^T + O_P(h^{-1-\epsilon d} n^{-\beta}), \\ \frac{1}{n} \sum_{i=1}^n \hat{\mathbf{x}}_i^T K_h(\|\hat{X}_i - \iota(x)\|) \hat{\mathbf{x}}_i &= \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^T K_h(\|X_i - x\|) \mathbf{x}_i + O_P(h^{-1-\epsilon d} n^{-\beta}). \end{aligned}$$

Therefore,

$$\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}} = \frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{X} + O_P(h^{-1-\epsilon d} n^{-\beta}) \mathbf{1}_{d \times 1} \mathbf{1}_{d \times 1}^T, \quad (28)$$

with

$$\frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{X} = \begin{bmatrix} n^{-1} \sum_{i=1}^n K_h(\|X_i - x\|) & n^{-1} \sum_{i=1}^n K_h(\|X_i - x\|) \mathbf{x}_i^T \\ n^{-1} \sum_{i=1}^n K_h(\|X_i - x\|) \mathbf{x}_i & n^{-1} \sum_{i=1}^n \mathbf{x}_i K_h(\|X_i - x\|) \mathbf{x}_i^T \end{bmatrix}.$$

By Lemma S.1, S.2 and S.3, we have

$$\begin{aligned} \frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{X} = & \begin{bmatrix} f(x) & h^2 u_{1,2} d^{-1} \nabla f(x)^T \\ h^2 u_{1,2} d^{-1} \nabla f(x) & h^2 u_{1,2} d^{-1} f(x) \mathbf{I}_d \end{bmatrix} \\ & + \begin{bmatrix} O(h^2) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}}) & O(h^3) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) \\ O(h^3) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) & O(h^{7/2}) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+2}) \end{bmatrix}, \end{aligned}$$

where $u_{q,k}$ are constants defined in Section S.2 of Supplementary Material. Therefore, combined with (28), it yields

$$\begin{aligned} \frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}} = & \begin{bmatrix} f(x) & h^2 u_{1,2} d^{-1} \nabla f(x)^T \\ h^2 u_{1,2} d^{-1} \nabla f(x) & h^2 u_{1,2} d^{-1} f(x) \mathbf{I}_d \end{bmatrix} \\ & + \begin{bmatrix} O(h^2) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}}) + O_P(h^{-1-\epsilon d} n^{-\beta}) & O(h^3) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) + O_P(h^{-1-\epsilon d} n^{-\beta}) \\ O(h^3) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) + O_P(h^{-1-\epsilon d} n^{-\beta}) & O(h^{7/2}) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+2}) + O_P(h^{-1-\epsilon d} n^{-\beta}) \end{bmatrix}. \end{aligned}$$

By our choice of h , we have $h^{-1-\epsilon d} n^{-\beta} \ll h^2$. Then, by binomial inverse theorem and matrix blockwise inversion, we have

$$\begin{aligned} \left(\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}} \right)^{-1} = & \begin{bmatrix} \frac{1}{f(x)} & -\frac{\nabla^T f(x)}{f(x)^2} \\ \frac{\nabla^T f(x)}{f(x)^2} & h^{-2} \frac{d}{u_{1,2} f(x)} \mathbf{I}_d \end{bmatrix} \\ & + \begin{bmatrix} O_P(h^2 + h^{-1-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}}) & O_P(h + h^{-3-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-1}) \\ O_P(h + h^{-3-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-1}) & O_P(h^{-\frac{1}{2}} + h^{-5-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-2}) \end{bmatrix}. \end{aligned} \quad (29)$$

Therefore, with (27), we conclude that

$$\mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \left\{ (\mathbf{X} - \hat{\mathbf{X}}) \begin{bmatrix} g(x) \\ \nabla g(x) \end{bmatrix} \right\} = O_P(h^{-1-\epsilon d} n^{-\beta}). \quad (30)$$

Now we analyze (26) with a focus on the term $\hat{\mathbf{X}}^T \hat{\mathbf{W}} \mathbf{H}$. A calculation similar to those in Lemma

S.3 and S.2 shows that

$$\frac{1}{n} \sum_{i=1}^n K_h(\|X_i - \iota(x)\|) \mathbf{x}_i^T \text{Hess } g(x) \mathbf{x}_i = h^2 u_{1,2} d^{-1} f(x) \Delta g(x) + O_P(h^{7/2} + n^{-1/2} h^{-d/2+2})$$

and

$$\frac{1}{n} \sum_{i=1}^n K_h(\|X_i - \iota(x)\|) \mathbf{x}_i^T \text{Hess } g(x) \mathbf{x}_i \mathbf{x}_i = O_P(h^4 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+3}).$$

Therefore,

$$\frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{H} = \begin{bmatrix} h^2 u_{1,2} d^{-1} f(x) \Delta g(x) + O_P(h^{7/2} + n^{-1/2} h^{-d/2+2}) \\ h^4 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+3} \end{bmatrix}$$

and hence

$$\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \mathbf{H} = \begin{bmatrix} h^2 u_{1,2} d^{-1} f(x) \Delta g(x) + O_P(h^{7/2} + n^{-1/2} h^{-d/2+2} + h^{-1-\epsilon d} n^{-\beta}) \\ O_P(h^4 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+3} + h^{-1-\epsilon d} n^{-\beta}) \end{bmatrix}.$$

The choice of h implies that $n^{-\frac{1}{2}} h^{-\frac{d}{2}} \ll 1$. Thus, with (29), we conclude that

$$\mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \left\{ \frac{1}{2} \mathbf{H} + O_P(h^3) \right\} = \frac{1}{2d} h^2 u_{1,2} \Delta g(x) + O_P(h^3 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+2} + h^{-1-\epsilon d} n^{-\beta}).$$

Combining the above equation with (26) and (30), we immediately see that the conditional bias is

$$\mathbf{E}\{\hat{g}(x) - g(x) \mid \mathcal{D}\} = \frac{1}{2d} h^2 u_{1,2} \Delta g(x) + O_P(h^3 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+2} + h^{-1-\epsilon d} n^{-\beta}). \quad (31)$$

Now we analyze the conditional variance. Simple calculation shows that

$$\begin{aligned} \mathbf{Var}\{\hat{g}(x) \mid \mathcal{D}\} &= \sigma_\zeta^2 \mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{W}} \hat{\mathbf{X}} (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \mathbf{e}_1^T \\ &= n^{-1} \sigma_\zeta^2 \mathbf{e}_1^T (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{W}} \hat{\mathbf{X}}) (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \mathbf{e}_1^T. \end{aligned} \quad (32)$$

It is easy to see that

$$\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{W}} \hat{\mathbf{X}} = \frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{W} \mathbf{X} + O_P(n^{-\beta} h^{-d-1-\epsilon d}) \mathbf{1}_{(d+1) \times (d+1)}. \quad (33)$$

Also,

$$\frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{W} \mathbf{X} = \begin{bmatrix} \frac{1}{n} \sum_{i=1}^n K_h^2(\|X_i - x\|) & \frac{1}{n} \sum_{i=1}^n K_h^2(\|X_i - x\|) \mathbf{x}_i^T \\ \frac{1}{n} \sum_{i=1}^n K_h^2(\|X_i - x\|) \mathbf{x}_i & \frac{1}{n} \sum_{i=1}^n K_h^2(\|X_i - x\|) \mathbf{x}_i \mathbf{x}_i^T \end{bmatrix}.$$

With Lemma S.1, S.2 and S.3, we can show that

$$\begin{aligned} \frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{W} \mathbf{X} &= h^{-d} \begin{bmatrix} u_{2,0} \sigma^2 f(x) & h^2 d^{-1} u_{2,2} \sigma^2 \nabla f(x) \\ h^2 d^{-1} u_{2,2} \sigma^2 \nabla^T f(x) & h^2 d^{-1} u_{2,2} \sigma^2 f(x) \mathbf{I}_d \end{bmatrix} \\ &\quad + h^{-d} \begin{bmatrix} O(h^2) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}}) & O_P(h^3 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) \\ O_P(h^3 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) & O_P(h^{\frac{7}{2}} + n^{-\frac{1}{2}} h^{-\frac{d}{2}+2}) \end{bmatrix}. \end{aligned}$$

Combined with (29), the above equation implies that

$$\begin{aligned} &n^{-1} \sigma_\epsilon^2 \mathbf{e}_1^T (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} (n^{-1} \mathbf{X}^T \mathbf{W} \mathbf{W} \mathbf{X}) (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \mathbf{e}_1^T \\ &= \frac{1}{n h^d} \frac{u_{2,0} \sigma_\zeta^2}{f(x)} + O_P \left(n^{-1} h^{-d} (h^{-1-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}}) \right). \end{aligned} \quad (34)$$

Also,

$$\begin{aligned} &n^{-1} \sigma_\zeta^2 \mathbf{e}_1^T (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \mathbf{1}_{(d+1) \times (d+1)} (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \mathbf{e}_1^T O_P(h^{-d-1-\epsilon d} n^{-\beta}) \\ &= n^{-1} O_P(1 + h + h^{-1-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-1}) O_P(h^{-d-1-\epsilon d} n^{-\beta}). \\ &= O_P \left(n^{-\beta-1} h^{-d-1-\epsilon d} (1 + h + h^{-1-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-1}) \right). \end{aligned} \quad (35)$$

Combining the above result with (32), (33), (34) and (35) gives the conditional variance

$$\begin{aligned} \mathbf{Var}\{\hat{g}(x) \mid \mathcal{D}\} &= \frac{1}{n h^d} \frac{u_{2,0} \sigma_\zeta^2}{f(x)} + O_P \left(n^{-1} h^{-d} (h^2 + h^{-1-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}}) \right) \\ &\quad + O_P \left(n^{-\beta-1} h^{-d-1-\epsilon d} (1 + h + h^{-1-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-1}) \right). \end{aligned}$$

The choice of h implies that $h^2 \geq h^{-1-\epsilon d} n^{-\beta}$. Therefore, the above asymptotic rate can be simplified to

$$\mathbf{Var}\{\hat{g}(x) \mid \mathcal{D}\} = \frac{1}{nh^d} \frac{u_{2,0}\sigma_\zeta^2}{f(x)} + O_P\left(n^{-1}h^{-d}(h + n^{-\frac{1}{2}}h^{-\frac{d}{2}})\right). \quad (36)$$

Finally, the rate for $\mathbf{E}[\{\hat{g}(x) - g(x)\}^2 \mid \mathcal{D}]$ is derived from (31) and (36). \square

References

- Bickel, P. J. and Li, B. (2007) Local polynomial regression on unknown manifolds. In *Complex Datasets and Inverse Problems: Tomography, Networks and Beyond*, Lecture Notes-Monograph Series, 177–186.
- Boucheron, S., Lugosi, G. and Massart, P. (2016) *Concentration Inequalities: A Nonasymptotic Theory of Independence*. Oxford, United Kingdom: Oxford University Press.
- Cai, T. and Yuan, M. (2011) Optimal estimation of the mean function based on discretely sampled functional data: Phase transition. *The Annals of Statistics*, **39**, 2330–2355.
- Cardot, H., Ferraty, F. and Sarda, P. (1999) Functional linear model. *Statistics & Probability Letters*, **45**, 11–22.
- (2003) Spline estimators for the functional linear model. *Statistica Sinica*, **13**, 571–591.
- Cardot, H. and Sarda, P. (2005) Estimation in generalized linear models for functional data via penalized likelihood. *Journal of Multivariate Analysis*, **92**, 24–41.
- Chen, D. and Müller, H. (2012) Nonlinear manifold representations for functional data. *The Annals of Statistics*, **40**, 1–29.
- Cheng, M. and Wu, H. (2013) Local linear regression on manifolds and its geometric interpretation. *Journal of the American Statistical Association*, **108**, 1421–1434.
- Cornea, E., Zhu, H., Kim, P. and Ibrahim, J. G. (2016) Regression models on Riemannian symmetric spaces. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, in press.
- Delaigle, A. and Hall, P. (2010) Defining probability density for a distribution of random functions. *The Annals of Statistics*, **38**, 1171–1193.
- Fan, J. (1992) Design-adaptive nonparametric regression. *Journal of the American Statistical Association*

- sociation*, **87**, 998–1004.
- (1993) Local linear regression smoothers and their minimax efficiencies. *The Annals of Statistics*, **21**, 196–216.
- Ferraty, F., Keilegom, I. V. and Vieu, P. (2012) Regression when both response and predictor are functions. *Journal of Multivariate Analysis*, **109**, 10–28.
- Ferraty, F. and Vieu, P. (2006) *Nonparametric Functional Data Analysis: Theory and Practice*. New York: Springer-Verlag.
- Gräf, M. and Potts, D. (2009) Sampling sets and quadrature formulae on the rotation group. *Journal of Numerical Functional Analysis and Optimization*, **30**, 665–688.
- Hall, P. and Horowitz, J. L. (2007) Methodology and convergence rates for functional linear regression. *The Annals of Statistics*, **35**, 70–91.
- Hall, P. and Hosseini-Nasab, M. (2006) On properties of functional principal components analysis. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **68**, 109–126.
- Hall, P. and Marron, J. S. (1997) On the shrinkage of local linear curve estimators. *Statistics and Computing*, **516**, 11–17.
- Hall, P., Müller, H. G. and Wang, J. L. (2006) Properties of principal component methods for functional and longitudinal data analysis. *The Annals of Statistics*, **34**, 1493–1517.
- Kong, D., Xue, K., Yao, F. and Zhang, H. H. (2016) Partially functional linear regression in high dimensions. *Biometrika*, **103**, 147–159.
- Kudraszow, N. L. and Vieu, P. (2013) Uniform consistency of kNN regressors for functional variables. *Statistics & Probability Letters*, **83**, 1863–1870.
- Lang, S. (1995) *Differential and Riemannian Manifolds*. New York: Springer.
- (1999) *Fundamentals of Differential Geometry*. New York: Springer.
- Levina, E. and Bickel, P. (2004) Maximum likelihood estimation of intrinsic dimension. *Advances in Neural Information*, **17**, 777–784.
- Li, Y. and Hsing, T. (2010) Uniform convergence rates for nonparametric regression and principal component analysis in functional/longitudinal data. *The Annals of Statistics*, **38**, 3321–3351.

- Lila, E. and Aston, J. (2017) Smooth principal component analysis over two-dimensional manifolds with an application to neuroimaging. *The Annals of Applied Statistics*. To appear, arXiv:1601.03670.
- Mas, A. (2012) Lower bound in regression for functional data by representation of small ball probabilities. *Electronic Journal of Statistics*, **6**, 1745–1778.
- Müller, H.-G. and Stadtmüller, U. (2005) Generalized functional linear models. *The Annals of Statistics*, **33**, 774–805.
- Müller, H.-G. and Yao, F. (2008) Functional additive models. *Journal of the American Statistical Association*, **103**, 1534–1544.
- Ramsay, J. O. and Silverman, B. (2002) *Applied Functional Data Analysis: Methods and Case Studies*. New York: Springer.
- Ramsay, J. O. and Silverman, B. W. (1997) *Functional Data Analysis*. New York: Springer-Verlag.
- (2005) *Functional Data Analysis*. Springer Series in Statistics. Springer, 2nd edn.
- Seifert, B. and Gasser, T. (1996) Finite-sample variance of local polynomials: analysis and solutions. *Journal of the American Statistical Association*, **91**, 267–275.
- Singer, A. and Wu, H.-T. (2012) Vector diffusion maps and the connection laplacian. *Communications on Pure and Applied Mathematics*, **65**, 1067–1144.
- Stuelpnagel, J. (1964) On the parametrization of the three-dimensional rotation group. *SIAM Review*, **6**, 422–430.
- Tsybakov, A. B. (2008) *Introduction to Nonparametric Estimation*. New York: Springer.
- Yao, F. and Müller, H.-G. (2010) Functional quadratic regression. *Biometrika*, **97**, 49–64.
- Yao, F., Müller, H.-G. and Wang, J.-L. (2005a) Functional data analysis for sparse longitudinal data. *Journal of the American Statistical Association*, **100**, 577–590.
- Yao, F., Müller, H.-G. and Wang, J.-L. (2005b) Functional linear regression analysis for longitudinal data. *The Annals of Statistics*, **33**, 2873–2903.
- Yuan, M. and Cai, T. T. (2010) A reproducing kernel Hilbert space approach to functional linear regression. *The Annals of Statistics*, **38**, 3412–3444.

- Yuan, Y., Zhu, H., Lin, W. and Marron, J. S. (2012) Local polynomial regression for symmetric positive definite matrices. *Journal of Royal Statistical Society: Series B (Statistical Methodology)*, **74**, 697–719.
- Zhang, X. and Wang, J.-L. (2016) From sparse to dense functional data and beyond. *The Annals of Statistics*, **44**, 2281–2321.
- Zhou, L. and Pan, H. (2014) Principal component analysis of two-dimensional functional data. *Journal of Computational and Graphical Statistics*, **23**, 779–801.

Supplementary Material

S.1. Auxiliary Results

For convenience, in the sequel we simplify $\mathcal{L}^2(D)$ by \mathcal{L}^2 , and use $\|\cdot\|$ to denote the norm $\|\cdot\|_{\mathcal{L}^2}$ when no confusion arises.

PROPOSITION S.1. *Let X be defined in Example 1. Suppose $\omega \in (a, b)$ with $|a - b| < 1$ and $v = (\cos 2\pi\omega, \sin 2\pi\omega)$. Then the embedded tangent space at $X(v)$ is given by $\text{span}\{\sum_k k^{-c} k \sin(2k\pi\omega)\phi_k\}$.*

PROOF. Let $V = \{(\cos 2\pi\omega, \sin 2\pi\omega) : \omega \in (a, b)\}$ be a local neighborhood of v , and let $\psi(v) = \omega \in (a, b)$ for $v = (v_1, v_2) = (\cos 2\pi\omega, \sin 2\pi\omega) \in V$. Then ψ is a chart of S^1 . Let U be open in \mathcal{L}^2 such that $X(v) \in U$. Since \mathcal{L}^2 is a linear space, the identity map \mathbf{I} serves as a chart. Let $X_{U,V} : \psi(V) \rightarrow \mathcal{L}^2$ denote the map $X \circ \psi^{-1}$. Let $\vartheta = -\sum_k 2\pi k^{-c+1} \sin(2k\pi\omega)\phi_k$. It defines a linear map from \mathbb{R} to \mathcal{L}^2 , denoted by $\Theta(t) = t\vartheta \in \mathcal{L}^2$. Then,

$$\begin{aligned} A(t) &\equiv t^{-2} \|X_{U,V}(\omega + t) - X_{U,V}(\omega) - t\vartheta\|^2 \\ &= t^{-2} \sum_{k=1}^{\infty} \{k^{-c} \cos(2k\pi(\omega + t)) - k^{-c} \cos(2k\pi\omega) + 2\pi k^{-c+1} \sin(2k\pi\omega)t\}^2 \\ &= t^{-2} \sum_{k=1}^{\infty} k^{-2c} [\cos(2k\pi\omega)\{\cos(2k\pi t) - 1\} + \sin(2k\pi\omega)\{2k\pi t - \sin(2k\pi t)\}]^2 \\ &\leq \sum_{k=1}^{\infty} 3k^{-2c} \left\{ \left| \frac{\cos(2k\pi t) - 1}{t} \right|^2 + 4k^2\pi^2 + \left| \frac{\sin(2k\pi t)}{t} \right|^2 \right\} \equiv \sum_{k=1}^{\infty} 3k^{-2c} B(t, k). \end{aligned}$$

By mean value theorem,

$$\left| \frac{\cos(2k\pi t) - 1}{t} \right| = 2k\pi \left| \frac{\cos(2k\pi t) - \cos(0)}{2k\pi t - 0} \right| \leq 2k\pi \sup_t |\sin(2k\pi t)| = 2k\pi.$$

Similarly, $|\sin(2k\pi t)|/|t| \leq 2k\pi$. Therefore, $0 \leq 3k^{-2c}B(t, k) \leq 36k^{-2c+2}\pi^2$. Since $\sum_{k=1}^{\infty} k^{-2c+2} < \infty$ for $c > 3/2$, we apply Dominated Convergence Theorem to conclude that

$$\lim_{t \rightarrow 0} A(t) = \sum_{k=1}^{\infty} \lim_{t \rightarrow 0} \{k^{-c} \cos(2k\pi(\omega + t)) - k^{-c} \cos(2k\pi\omega) + 2\pi k^{-c+1} \sin(2k\pi\omega)t\}^2 = 0.$$

This shows that ϑ is an embedded tangent vector at $X(v)$, and the conclusion of the proposition follows. \square

Next result asserts that the local neighborhood based on contaminated data \hat{X}_i is indeed close to that based on true X_i with large probability.

PROPOSITION S.2. *Define $h_- = h_{pca} - n^{-(\beta+\varrho)/2}$ and $h_+ = h_{pca} + n^{-(\beta+\varrho)/2}$. Let $Z_i = 1_{\{\hat{X}_i \in \mathbb{B}_{h_{pca}}^{\mathcal{L}^2}(x)\}}$, $V_{i0} = 1_{\{X_i \in \mathbb{B}_{h_-}^{\mathcal{L}^2}(x)\}}$ and $V_{i1} = 1_{\{X_i \in \mathbb{B}_{h_+}^{\mathcal{L}^2}(x)\}}$. Under assumption (B3) in the paper, then $\Pr(\forall i : V_{i0} \leq Z_i \leq V_{i1}) \rightarrow 1$, $n \rightarrow \infty$.*

Hence one can always obtain lower and upper bounds for quantities involving Z_i in terms of V_{i0} and V_{i1} , i.e., with large probability, it is equivalent to substitute Z_i with V_{i0} and V_{i1} in our analysis.

PROOF. We first bound the following event

$$\begin{aligned} \Pr(\forall i : Z_i \leq V_{i1}) &= \prod_{i=1}^n \{1 - \Pr(Z_i > V_{i1})\} = \{1 - \Pr(Z > V_1)\}^n \\ &= \{1 - \Pr(Z = 1, V_1 = 0)\}^n \geq \left\{1 - \Pr(\|\hat{X} - X\| \geq n^{-(\beta+\varrho)/2})\right\}^n \\ &\geq \left(1 - c_1^p n^{p(\beta+\varrho)/2} n^{-p\beta}\right)^n \geq (1 - c_1^p n^{-2})^n \rightarrow 1, \end{aligned}$$

where $c_1 > 0$ is some constant, and $p > 0$ is a constant that is sufficiently large so that $p(\beta - \varrho) \geq 4$. Similarly, we can deduce that

$$\Pr(\forall i : V_{i0} \leq Z_i) \rightarrow 1,$$

and the conclusion $\Pr(\forall i : V_{i0} \leq Z_i \leq V_{i1}) \rightarrow 1$ follows. \square

S.2. Technical Lemmas

Here we collect some technical lemmas that will be used in the proofs of Theorems in the paper. First, let us establish some notations. Let $u_{q,k} = \int_{\mathbb{B}_1^{\mathbb{R}}(0)} K^q(\|u\|_{\mathbb{R}^d}) \|u\|_{\mathbb{R}^d}^k du$. We also identify $\iota_* T_x \mathcal{M}$ with \mathbb{R}^d . Let $\mathbb{D}_{x,h}$ denote the set $\{\theta \in \mathbb{R}^d : \exp_x(\theta) \in \mathbb{B}_h^{\mathcal{M}}(x)\}$, where \exp_x denotes the exponential map at x . Let $\kappa_{11,q} = \int_{h^{-1}\mathbb{D}_{x,h}} K^q(\|u\|_{\mathbb{R}^d}) du$, $\kappa_{12,q,j} = \int_{h^{-1}\mathbb{D}_{x,h}} K^q(\|u\|_{\mathbb{R}^d}) \theta_j du$ and $\kappa_{22,q,j,k} = \int_{h^{-1}\mathbb{D}_{x,h}} K^q(h^{-1}\|\theta\|_{\mathbb{R}^d}) \theta_j \theta_k d\theta$, where θ_j denotes the j th component of θ . Let π_{d-1} denote the volume of the unit sphere S^{d-1} . The following three lemmas are based on Lemma A.2.5 of Cheng and Wu (2013) and hence their proofs are omitted.

LEMMA S.1. *Suppose K is a kernel function compactly supported in $[-1, 1]$ and continuously differentiable in $[0, 1]$. Let $h \geq h_{pca}$.*

(a) *If $x \in \mathcal{M} \setminus \mathcal{M}_h$, then*

$$n^{-1} \sum_{i=1}^n h^{-d} K^q \left(\frac{\|X_i - x\|_{\mathcal{L}^2}}{h} \right) = u_{q,0} f(x) + O(h^2) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}})$$

(b) *If $x \in \mathcal{M}_h$, then*

$$n^{-1} \sum_{i=1}^n h^{-d} K^q \left(\frac{\|X_i - x\|_{\mathcal{L}^2}}{h} \right) = f(x) \kappa_{11,q} + O(h) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}}).$$

LEMMA S.2. *Suppose K is a kernel function compactly supported in $[-1, 1]$ and continuously differentiable in $[0, 1]$. Let $h \geq h_{pca}$ and $\hat{\varphi}_k$ be the estimate in Theorem 2. Then,*

(a) *if $x \in \mathcal{M} \setminus \mathcal{M}_h$,*

$$\begin{aligned} & \frac{1}{n} \sum_{i=1}^n h^{-d} K^q \left(\frac{\|X_i - x\|_{\mathcal{L}^2}}{h} \right) \langle X_i - x, \hat{\varphi}_k \rangle \\ &= h^2 u_{q,1} d^{-1} \nabla_{\phi_k} f(x) + O_P(h^3 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+1} + h^2 h_{pca}^{3/2} + h^3 h_{pca}). \end{aligned}$$

(b) if $x \in \mathcal{M}_h$,

$$\frac{1}{n} \sum_{i=1}^n h^{-d} K^q \left(\frac{\|X_i - x\|_{\mathcal{L}^2}}{h} \right) \langle X_i - x, \hat{\varphi}_k \rangle = h\kappa_{12,q,k}(x) + O_P(h^2 + n^{-\frac{1}{2}}h^{-\frac{d}{2}+1} + hh_{pca}^{3/2} + h^2h_{pca}).$$

LEMMA S.3. Suppose K is a kernel function compactly supported in $[-1, 1]$ and continuously differentiable in $[0, 1]$. Let $h \geq h_{pca}$.

(a) If $x \in \mathcal{M} \setminus \mathcal{M}_h$, then

$$\begin{aligned} & n^{-1} \sum_{i=1}^n h^{-d} K^q \left(\frac{\|X_i - x\|_{\mathcal{L}^2}}{h} \right) \langle X_i - x, \hat{\varphi}_j \rangle \langle X_i - x, \hat{\varphi}_k \rangle \\ &= \begin{cases} h^2 u_{q,2} d^{-1} f(x) + O_P(h^{\frac{7}{2}} + n^{-\frac{1}{2}}h^{-\frac{d}{2}+2}) & \text{if } 1 \leq j = k \leq d \\ O_P(h^{\frac{7}{2}} + n^{-\frac{1}{2}}h^{-\frac{d}{2}+2}) & \text{otherwise.} \end{cases} \end{aligned}$$

(b) If $x \in \mathcal{M}_h$, then

$$\begin{aligned} & n^{-1} \sum_{i=1}^n h^{-d} K^q \left(\frac{\|X_i - x\|_{\mathcal{L}^2}}{h} \right) \langle X_i - x, \hat{\varphi}_j \rangle \langle X_i - x, \hat{\varphi}_k \rangle \\ &= h^2 f(x) \kappa_{22,q,j,k}(x) + O_P(h^3 + n^{-\frac{1}{2}}h^{-\frac{d}{2}+2} + h^2h_{pca}^{3/2}). \end{aligned}$$

The following two lemmas are used in proving Theorem 1.

LEMMA S.4. Suppose V_1, V_2, \dots, V_N are i.i.d. random variables with mean zero. Assume $\mathbf{E}V^r \leq a^r h^{1-r} + b^r h^{\kappa r}$ for some constants $a, b, \kappa \geq 0$ and $r \geq 2$. Suppose $h \geq N^{-1}$. Then, for any integer $p \geq 1$, we have

$$\mathbf{E} \left\{ \left(\frac{1}{N} \sum_{j=1}^N V_j \right)^{2p} \right\} \leq (2p)^{p-1} (2p)! p 2^p (a^{2p} + b^{2p}) N^{-p} h^{-p}.$$

PROOF. By multinomial theorem,

$$\left(\sum_{j=1}^N V_j \right)^{2p} = \sum_{k_1 + \dots + k_N = 2p} \binom{2p}{k_1, k_2, \dots, k_N} \prod_{j=1}^N V_j^{k_j}.$$

For each $\prod_{j=1}^N V_j^{k_j}$, if $k_j = 1$ for some j , then it is zero. Let $S(k_1, \dots, k_N)$ denote the number of non-zero k_j . Then, there are in total $\binom{N}{1}$ items such that $S(k_1, \dots, k_N) = 1$, at most $\binom{N}{2}(2p)$ items such that $S(k_1, \dots, k_N) = 2$, etc. In fact, there are at most $\binom{N}{q}(2p)^{q-1}$ items such that $S(k_1, \dots, k_N) = q$, for every $q \leq p$. Note that by assumption, $\mathbf{E}V^r \leq a^r h^{1-r} + b^r h^{\nu_{\kappa} r} \leq (a^r + b^r)h^{1-r}$ for $r \geq 2$. Therefore,

$$\begin{aligned} \mathbf{E} \left(\sum_{j=1}^N V_j \right)^{2p} &\leq \sum_{q=1}^p \binom{N}{q} (2p)^{q-1} \binom{2p}{k_1, k_2, \dots, k_N} 2^q (a^{2p} h^{q-2p} + b^{2p} h^{q-2p}) \\ &\leq (2p)^{p-1} (2p)! 2^p (a^{2p} + b^{2p}) \sum_{q=1}^p \frac{N!}{(N-q)! q!} h^{q-2p} \\ &\leq (2p)^{p-1} (2p)! p 2^p (a^{2p} + b^{2p}) \sum_{q=1}^p N^p h^{q-2p} \\ &\leq (2p)^{p-1} (2p)! p 2^p (a^{2p} + b^{2p}) N^p h^{-p}. \end{aligned}$$

Multiplying both sides by N^{-2p} yields the conclusion of the lemma. \square

LEMMA S.5. Suppose $D \subset \mathbb{R}^p$ is compact set and $S_N(t)$ for $t \in D$ is a sequence of random processes defined on D . For $b_N > 0$, define $\delta_N(t) = 2b_N 1_{\{|S(t)| \leq b_N\}}$. Suppose for some constant c_0 , $0 < c_0 \leq \mathbf{E}S_N(t) < \infty$ for all t and sufficiently large N . Also, assume $\lim_{N \rightarrow \infty} \inf_{t \in D} \mathbf{E}S_N(t) > 0$. For a sequence of $a_N \rightarrow 0$ and any $p > 0$, if $b_N^{-r} a_N^p \leq 1$ for some p and $r > 0$, and

(a) if $\mathbf{E}(\sup_{t \in D} |S_N(t) - \mathbf{E}S(t)|^p) = O(a_N^p)$, then we have

$$\mathbf{E} \sup_{t \in D} \left| \frac{1}{S_N(t) + \delta_N(t)} - \frac{1}{\mathbf{E}S_N(t)} \right|^r = O(a_N^r + b_N^r);$$

(b) if $\int_D \mathbf{E}(|S_N(t) - \mathbf{E}S_N(t)|^p) dt = O(a_N^p)$, then we have

$$\mathbf{E} \int \left| \frac{\mathbf{E}S_N(t)}{S_N(t) + \delta_N(t)} - 1 \right|^r dt = O(a_N^r + b_N^r).$$

PROOF. From now on, we shall suppress N when there is no confusion raised. Let $\tilde{S}(t) =$

$S(t) + \delta(t)$ and $v(t) = \mathbf{E}\tilde{S}(t) - \mathbf{E}\delta(t) = \mathbf{E}S(t)$. For a fixed t that is suppressed below,

$$\begin{aligned}
\left| \frac{v}{\tilde{S}} - 1 \right|^r &\leq \left(\frac{|\tilde{S} - v|^r}{|\tilde{S}|^r} \right) 1_{\{|\tilde{S} - v| \leq v/2\}} + \left(\frac{|\tilde{S} - v|^r}{|\tilde{S}|^r} \right) 1_{\{|\tilde{S} - v| > v/2\}} \\
&\leq (v/2)^{-r} \left| \tilde{S} - v \right|^r + b_N^{-r} \left| \tilde{S} - v \right|^r 1_{\{|\tilde{S} - v| > v/2\}} \\
&\leq c_r (v/2)^{-r} |S - \mathbf{E}S|^r + c_r (v/2)^{-r} \delta^r + b_N^{-r} \left| \tilde{S} - v \right|^r 1_{\{|\tilde{S} - v| > v/2\}} \\
&\equiv I_1 + I_2 + I_3,
\end{aligned}$$

where $c_r > 0$ is a constant independent of t .

(a) By assumption, $\mathbf{E} \sup_t I_1 = O(a_N^r)$. Since $|\delta| \leq 2b_N$, we have $\mathbf{E} \sup_t I_2 = O(b_N^r)$. Also,

$$\mathbf{E} \sup_t I_3 \leq c_p b_N^{-r} \sup_t (v/2)^{-p} \mathbf{E}(\sup_t |S - v|^{p+r} + \sup_t |\delta|^{p+r}) = O(b_N^{-r} a_N^{p+r}) = O(a_N^r + b_N^r)$$

for sufficiently large p , and a constant $c_p > 0$.

(b) By assumption, $\int I_1 dt = O(a_N^r)$. Since $|\delta| \leq 2b_N$, we have $\int I_2 dt = O(b_N^r)$. Also,

$$\int I_3 dt \leq b_N^{-r} \int \{v(t)/2\}^{-p} \mathbf{E}|\tilde{S}(t) - v(t)|^{p+r} dt = O(b_N^{-r} a_N^{p+r}) = O(a_N^r + b_N^r).$$

Therefore, the conclusion of part (b) follows. □

In order to prove Theorem 2, we establish the following auxiliary lemmas.

LEMMA S.6. *Let $\tilde{G} = \hat{G} + \Delta$ with $\Delta = 1/\log n$. Then $\mathbf{E}|\log \tilde{G} - \log G| = o(1)$.*

PROOF. By Jensen's inequality and concavity of $\log(\cdot)$,

$$\begin{aligned}
\mathbf{E}(\log \tilde{G} - \log G) &\leq \log \mathbf{E} \frac{\tilde{G}}{G} = \log \mathbf{E} \frac{\|X - x\|}{\|\hat{X} - x\| + \Delta} \leq \log \mathbf{E} \frac{\|\hat{X} - x\| + \|\hat{X} - X\|}{\|\hat{X} - x\| + \Delta} \\
&\leq \log(1 + \Delta^{-1} \mathbf{E}\|\hat{X} - X\|) \equiv a_n
\end{aligned}$$

with $a_n \geq 0$ and $a_n \rightarrow 0$. For other other direction, we first observe that

$$\begin{aligned}
\mathbf{E} \left(\frac{\tilde{G}}{G} \right)^{1/4} &= \mathbf{E} \left\{ \frac{1}{G^{1/4}} \mathbf{E}(\tilde{G}^{1/4} \mid X) \right\} \leq \mathbf{E} \left\{ \frac{1}{G^{1/4}} \mathbf{E}(\|\hat{X} - X\|^{1/4} + \|X - x\|^{1/4} + \Delta^{1/4} \mid X) \right\} \\
&\leq \mathbf{E} \left[\frac{C_1^{1/4} n^{-\beta/4} \{\eta(X)\}^{1/4} + \Delta^{1/4} + G^{1/4}}{G^{1/4}} \right] \\
&\leq 1 + \left(\mathbf{E} G^{-1/2} \mathbf{E} \left[C_1^{1/4} n^{-\beta/4} \{\eta(X)\}^{1/4} + \Delta^{1/4} \right]^2 \right)^{1/2} \\
&\leq 1 + \left(\mathbf{E} G^{-1/2} \right)^{1/2} 2^{1/2} \left(\mathbf{E} \left[C_1^{1/2} n^{-\beta/2} \{\eta(X)\}^{1/2} + \Delta^{1/2} \right] \right)^{1/2} \\
&\leq 1 + O(n^{-\beta/4} + (\log n)^{-1/4})
\end{aligned}$$

where $C_1 > 0$ is some constant. This implies that

$$\frac{1}{4} \mathbf{E}(\log G - \log \tilde{G}) = \mathbf{E} \log \left(\frac{\tilde{G}}{G} \right)^{1/4} \leq \log \mathbf{E} \left(\frac{\tilde{G}}{G} \right)^{1/4} \equiv \frac{b_n}{4}$$

with $b_n \geq 0$ and $b_n \rightarrow 0$, or equivalently,

$$\mathbf{E}(\log \tilde{G} - \log G) \geq -b_n.$$

Therefore $\mathbf{E}|\log \tilde{G} - \log G| \leq a_n + b_n = o(1)$. □

LEMMA S.7. Suppose $0 < a < \beta$, $h \asymp n^{-a}$ and $h_+ = h + n^{-(\beta+a)/2}$. Let $Z = 1_{\{\hat{X} \in \mathbb{B}_h^{\mathcal{L}^2}(x)\}}$ and $V = 1_{\{X \in \mathbb{B}_{h_+}^{\mathcal{L}^2}(x)\}}$. If F is a positive functional of X and \hat{X} such that $\mathbf{E}\{F(X, \hat{X})V\} = O(h^b)$ for some $b \geq 0$, and $\mathbf{E}\{F(X, \hat{X})\} < \infty$ for some $q > 1$, then we have $\mathbf{E}\{F(X, \hat{X})|Z - V|\} = O(h^b)$ and $\mathbf{E}\{F(X, \hat{X})Z\} = O(h^b)$.

PROOF. Let $h_- = h - n^{-(\beta+a)/2}$ and $U = 1_{\{X \in \mathbb{B}_{h_-}^{\mathcal{L}^2}(x)\}}$. Note that $U \leq V$. Choose $r > 1$ such that $r^{-1} + q^{-1} = 1$. To reduce notational burden, we simply use F to denote $F(X, \hat{X})$. Then, by

Hölder inequality, we have

$$\begin{aligned}
\mathbf{E}(F|Z - V|) &= \mathbf{E}(F1_{Z=1}1_{V=0}) + \mathbf{E}(F1_{Z=0}1_{U=1}) + \mathbf{E}(F1_{Z=0}1_{V=1}1_{U=0}) \\
&\leq \mathbf{E}(F1_{Z=1}1_{V=0}) + \mathbf{E}(F1_{Z=0}1_{U=1}) + \mathbf{E}(FV) \\
&\leq (\mathbf{E}F^q)^{1/q} \left\{ (\mathbf{E}1_{Z=1}1_{V=0})^{1/r} + (\mathbf{E}1_{Z=0}1_{U=1})^{1/r} \right\} + \mathbf{E}(FV) \\
2 &\leq (\mathbf{E}F^q)^{1/q} \{ \Pr(\|X - \hat{X}\| \geq n^{-(\beta+a)/2}) \}^{1/r} + O(h^b) \\
2 &\leq (\mathbf{E}F^q)^{1/q} \left(n^{s(\beta+a)/2} \mathbf{E}\|X - \hat{X}\|^s \right)^{1/r} + O(h^b) \\
&\leq O\left(n^{s(\beta+a)/(2r) - s\beta/r}\right) + O(h^b),
\end{aligned}$$

where we choose $s \geq 2rab/(\beta - a)$ so that $n^{s(\beta+a)/(2r) - s\beta/r} \leq h^b$, and hence conclude that $\mathbf{E}(F|Z - V|) = O(h^b)$. Since $|\mathbf{E}(FZ) - \mathbf{E}(FV)| \leq \mathbf{E}(F|Z - V|)$, the result $\mathbf{E}(FZ) = O(h^b)$ follows. \square

LEMMA S.8. Suppose $\{\psi_k\}_{k=1}^\infty$ is an orthonormal basis of \mathcal{H} and $x \in \mathcal{M}$ is fixed. Assume that $\{\psi_1, \dots, \psi_d\}$ span the tangent space $\iota_* T_x \mathcal{M}$. Let π_{d-1} be the volume of the $d-1$ dimensional unit sphere S^{d-1} and $\hat{\mathcal{C}}_x$ the sample covariance operator based on $\hat{\mathcal{N}}_{\mathcal{L}^2}(h, x)$ for some $h \asymp n^{-a}$ with $0 < a < \beta$. Then,

$$\begin{aligned}
\sup_{j \leq d} \sup_{k \geq d+1} \left| \langle \hat{\mathcal{C}}_x \psi_j, \psi_k \rangle \right| &= O_P \left(h^{d+4} \log n + n^{-1/2} h^{d/2+3} + n^{-\beta} h^{d+1} \right), \\
\sup_{j, k \geq d+1} \left| \langle \hat{\mathcal{C}}_x \psi_j, \psi_k \rangle \right| &= O_P \left(h^{d+4} + n^{-1/2} h^{d/2+4} + n^{-\beta} h^{d+1} \right), \\
\sup_{1 \leq j \neq k \leq d} \left| \langle \hat{\mathcal{C}}_x \psi_j, \psi_k \rangle \right| &= O_P \left(h^{d+3} + n^{-1/2} h^{d/2+3} + n^{-\beta} h^{d+1} \right), \\
\text{for } 1 \leq k \leq d : \quad \langle \hat{\mathcal{C}}_x \psi_k, \psi_k \rangle &= \pi_{d-1} f(x) d^{-1} h^{d+2} + O_P \left(n^{-1/2} h^{d/2+2} + n^{-\beta} h^{d+1} \right).
\end{aligned}$$

PROOF. Denote $Z_i = 1_{\{\hat{X}_i \in \mathbb{B}_h^2(x)\}}$. Then $\hat{\mathcal{C}}$ can be written as $\hat{\mathcal{C}} = n^{-1} \sum_{i=1}^n (\hat{X}_i - \hat{\mu}_x) \otimes (\hat{X}_i -$

$\hat{\mu}_x)Z_i$. For any y, z such that $\|y\|_{\mathcal{L}^2} = \|z\|_{\mathcal{L}^2} = 1$, we have

$$\begin{aligned}
\langle \hat{\mathcal{C}}_x y, z \rangle &= \langle n^{-1} \sum_{i=1}^n Z_i (\hat{X}_i - \hat{\mu}_x) \otimes (\hat{X}_i - \hat{\mu}_x) y, z \rangle = n^{-1} \sum_{i=1}^n \langle \hat{X}_i - \hat{\mu}_x, y \rangle \langle \hat{X}_i - \hat{\mu}_x, z \rangle Z_i \\
&= n^{-1} \sum_{i=1}^n \langle X_i - \mu_x, y \rangle \langle X_i - \mu_x, z \rangle Z_i + n^{-1} \sum_{i=1}^n \langle (\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x), y \rangle \langle \hat{X}_i - \hat{\mu}_x, z \rangle Z_i \\
&\quad + n^{-1} \sum_{i=1}^n \langle \hat{X}_i - \hat{\mu}_x, y \rangle \langle (\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x), z \rangle Z_i \\
&\quad + n^{-1} \sum_{i=1}^n \langle (\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x), y \rangle \langle (\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x), z \rangle Z_i \\
&\equiv I_1 + I_2 + I_3 + I_4,
\end{aligned}$$

where $\mu_x = \sum_{i=1}^n X_i Z_i$ and $\hat{\mu}_x = \sum_{i=1}^n \hat{X}_i Z_i$. Before we proceed to analyze I_1, I_2, I_3 and I_4 , we prepare some calculations.

First, it is easy to check that

$$\|\hat{\mu}_x - \mu_x\| = \left\| \frac{1}{n} \sum_{i=1}^n \{(X_i - \mu_x) + (\hat{X}_i - X_i)\} Z_i \right\| \leq \frac{1}{n} \sum_{i=1}^n \|\hat{X}_i - X_i\| Z_i.$$

This implies that

$$\sum_{i=1}^n \|\hat{\mu}_x - \mu_x\| Z_i \leq \sum_{i=1}^n \|\hat{\mu}_x - \mu_x\| \leq \sum_{i=1}^n \|\hat{X}_i - X_i\| Z_i \quad (\text{S.1})$$

and

$$\sum_{i=1}^n \|\hat{\mu}_x - \mu_x\|^2 Z_i \leq \sum_{i=1}^n \|\hat{\mu}_x - \mu_x\|^2 \leq 2 \sum_{i=1}^n \|\hat{X}_i - X_i\|^2 Z_i. \quad (\text{S.2})$$

Now we analyze I_2 . It is seen that

$$\begin{aligned}
\mathbf{E} \sup_{y,z} |I_2| &\leq \mathbf{E} \sup_{y,z} \left| n^{-1} \sum_{i=1}^n \langle (\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x), y \rangle \langle \hat{X}_i - \hat{\mu}_x, z \rangle Z_i \right| \\
&\leq \mathbf{E} \sup_{y,z} n^{-1} \sum_{i=1}^n \|(\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x)\| \|\hat{X}_i - \hat{\mu}_x\| Z_i \\
&\leq \mathbf{E} \sup_{y,z} n^{-1} \sum_{i=1}^n \|(\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x)\| h Z_i \\
&\leq n^{-1} h \mathbf{E} \sum_{i=1}^n \left(\|\hat{X}_i - X_i\| + \|\hat{\mu}_x - \mu_x\| \right) Z_i \\
&\leq 2h \mathbf{E} \left(\|\hat{X}_i - X_i\| Z_i \right), \tag{S.3}
\end{aligned}$$

where the second inequality follows from Cauchy-Schwarz inequality and $\|y\|_{\mathcal{L}^2} = \|z\|_{\mathcal{L}^2} = 1$, the third one is from the fact that $\hat{\mu}_x, \hat{X}_i \in \mathbb{B}_h^{\mathcal{L}^2}(x)$ for $Z_i = 1$, the fourth one follows from triangle inequality, the fifth inequality is based on (S.1). Now, let $h_1 = h + n^{-(\beta+a)/2}$ and $V_i = 1_{\{X_i \in \mathbb{B}_{h_1}^{\mathcal{L}^2}(x)\}}$. Based on assumption (B3), $\mathbf{E}(\|\hat{X}_i - X_i\| V_i) = O(n^{-\beta} h_1^{d+1})$. Then, by Lemma S.7, $\mathbf{E}(\|\hat{X}_i - X_i\| Z_i) = O(n^{-\beta} h_1^{d+1}) = O(n^{-\beta} h^{d+1})$, since $h_1 \asymp h$. With (S.3), this shows that $\mathbf{E} \sup_{y,z} |I_2| = O(n^{-\beta} h^{d+1})$. Similarly, $\mathbf{E} \sup_{y,z} |I_3| = O(n^{-\beta} h^{d+1})$.

For I_4 , we have

$$\begin{aligned}
\mathbf{E} \sup_{y,z} |I_4| &= \mathbf{E} \sup_{y,z} n^{-1} \left| \sum_{i=1}^n \langle (\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x), y \rangle \langle (\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x), z \rangle Z_i \right| \\
&\leq \mathbf{E} \sup_{y,z} n^{-1} \sum_{i=1}^n \|(\hat{X}_i - X_i) - (\hat{\mu}_x - \mu_x)\|^2 Z_i \leq 2\mathbf{E} n^{-1} \sum_{i=1}^n (\|\hat{X}_i - X_i\|^2 + \|\hat{\mu}_x - \mu_x\|^2) Z_i \\
&\leq 4\mathbf{E} n^{-1} \sum_{i=1}^n \|\hat{X}_i - X_i\|^2 Z_i = 4\mathbf{E}(\|\hat{X}_i - X_i\|^2 Z_i),
\end{aligned}$$

where the first inequality comes from Cauchy-Schwarz inequality and $\|y\|_{\mathcal{L}^2} = \|z\|_{\mathcal{L}^2} = 1$, the second one follows from triangle inequality, and the third one is based on (S.2). By Lemma S.7, we can show that $\mathbf{E}(\|\hat{X}_i - X_i\|^2 Z_i) = O(n^{-2\beta} h^d)$.

The order of I_1 is given in Lemma S.9. Therefore, results of the lemma follow. \square

LEMMA S.9. For $0 < a < \beta$, let $h \asymp n^{-a}$ and $h_1 = h + n^{-(\beta+a)/2}$. Denote $Z_i = 1_{\{\hat{X}_i \in \mathbb{B}_h^{\mathcal{L}^2}(x)\}}$ and $\Xi_{j,k} = n^{-1} \sum_{i=1}^n \langle X_i - \mu_x, \psi_j \rangle \langle X_i - \mu_x, \psi_k \rangle Z_i$, where $\{\psi_k\}$ are defined in Lemma S.8. Then, we have

$$\mathbf{E} \sup_{j \leq d} \sup_{k \geq d+1} |\Xi_{j,k}| = O(h^{d+3}), \quad (\text{S.4})$$

$$\mathbf{E} \sup_{j,k \geq d+1} |\Xi_{j,k}| = O(h^{d+4}), \quad (\text{S.5})$$

$$\text{for } 1 \leq j \neq k \leq d : \quad \mathbf{E} \Xi_{j,k} = O(h^{d+3}), \quad (\text{S.6})$$

$$\text{for } 1 \leq k \leq d : \quad \mathbf{E} \Xi_{k,k} = O(h^{d+2}). \quad (\text{S.7})$$

Also,

$$\mathbf{Var} \left(\sup_{j \leq d} \sup_{k \geq d+1} |\Xi_{j,k}| \right) = O(n^{-1} h^{d+6}), \quad (\text{S.8})$$

$$\mathbf{Var} \left(\sup_{j,k \geq d+1} |\Xi_{j,k}| \right) = O(n^{-1} h^{d+8}),$$

$$\text{for } 1 \leq j \neq k \leq d : \quad \mathbf{Var} (|\Xi_{j,k}|) = O(n^{-1} h^{d+6}),$$

$$\text{for } 1 \leq k \leq d : \quad \mathbf{Var} (\Xi_{k,k}) = O(n^{-1} h^{d+4}).$$

PROOF. Let $V_i = 1_{\{X_i \in \mathbb{B}_{h_1}^{\mathcal{L}^2}(x)\}}$. Since $h_1 \asymp h$, we shall use them exchangeably when no confusion arises. Let \mathcal{P}_1 be projection into $\{\psi_1, \dots, \psi_d\}$ and \mathcal{P}_2 be projection into $\{\psi_{d+1}, \dots\}$.

First, for $1 \leq j \leq d$,

$$\begin{aligned}
\mathbf{E} \sup_{k \geq d+1} |\Xi_{j,k}| &\leq \mathbf{E} \sup_{k \geq d+1} \left| n^{-1} \sum_{i=1}^n \langle X_i - \mu_x, \psi_j \rangle \langle X_i - \mu_x, \psi_k \rangle Z_i \right| \\
&\leq \mathbf{E} \sup_{k \geq d+1} \left| n^{-1} \sum_{i=1}^n \langle X_i, \psi_j \rangle \langle X_i, \psi_k \rangle Z_i \right| \\
&\quad + \mathbf{E} \sup_{k \geq d+1} \left| n^{-1} \sum_{i=1}^n \langle \mu_x, \psi_j \rangle \langle \mu_x, \psi_k \rangle Z_i \right| \\
&= c_1(I_1 + I_2).
\end{aligned} \tag{S.9}$$

It is easy to see that I_1 is the dominant term, which we evaluate below (utilizing the fact that $\Pi_x(\theta, \theta) \perp T_x \mathcal{M}$):

$$\begin{aligned}
I_1 &= \mathbf{E} \sup_{k \geq d+1} \left| n^{-1} \sum_{i=1}^n \langle X_i, \psi_j \rangle \langle X_i, \psi_k \rangle Z_i \right| \leq \frac{1}{n} \mathbf{E} \sum_{i=1}^n \sup_{k \geq d+1} |\langle X_i, \psi_j \rangle \langle X_i, \psi_k \rangle Z_i| \\
&= \mathbf{E} \sup_{k \geq d+1} |\langle X_i, \psi_j \rangle \langle X_i, \psi_k \rangle Z_i| = \mathbf{E} \sup_{k \geq d+1} |\langle X_i, \psi_j \rangle \langle \mathcal{P}_2 X_i, \psi_k \rangle Z_i|. \\
&\leq \mathbf{E} (|\langle X_i, \psi_j \rangle| \|\mathcal{P}_2 X_i\| |Z_i|).
\end{aligned} \tag{S.10}$$

Since by Lemma A.2.4 of Cheng and Wu (2013),

$$\begin{aligned}
&\mathbf{E} |\langle X_i, \psi_j \rangle| \|\mathcal{P}_2 X_i\| |V_i| \\
&\leq \int_{S^{d-1}} \int_0^{h_1} \langle t\iota_* \theta, \psi_j \rangle \|t^2 \Pi_x(\theta, \theta)\|_{\mathcal{L}^2} f(\exp(t\theta)) t^{d-1} dt d\theta + O(h^{d+5}) \\
&= O(h^{d+3}),
\end{aligned}$$

we can apply Lemma S.7 to conclude $\mathbf{E} (|\langle X_i, \psi_j \rangle| \|\mathcal{P}_2 X_i\| |Z_i|) = O(h^{d+3})$, and hence with (S.10), we assert that $I_1 = O(h^{d+3})$. This proves (S.4). The result (S.5) is obtained in a similar way.

For (S.6), by the same argument of obtaining (S.9), we can show that for $1 \leq j \neq k \leq d$, $\mathbf{E} \Xi_{j,k}$

is dominated by

$$\mathbf{E} n^{-1} \sum_{i=1}^n \langle X_i, \psi_j \rangle \langle X_i, \psi_k \rangle Z_i = \mathbf{E} \langle X_i, \psi_j \rangle \langle X_i, \psi_k \rangle Z_i.$$

Now, because

$$\begin{aligned} & \mathbf{E} \langle X_i, \psi_j \rangle \langle X_i, \psi_k \rangle V_i \\ &= \int_{S^{d-1}} \int_0^{h_1} \langle t\iota_*\theta, \psi_j \rangle \langle t\iota_*\theta, \psi_k \rangle [f(x) + t\nabla_\theta f(x)] t^{d-1} dt d\theta + O(h^{d+4}) \\ &= O(h^{d+3}), \end{aligned}$$

where the second equality is based on the fact that the second fundamental form is self-adjoint, by Lemma S.7, (S.6) follows. The result (S.7) is dervied in a similar fashion.

Let $\chi_{i,k} = n^{-1} \langle X_i, \psi_j \rangle \langle X_i, \psi_k \rangle Z_i$. Then $\Xi_{j,k} = \sum_{i=1}^n \chi_{i,k}$. Then by Theorem 11.1 of Boucheron et al. (2016), we have

$$\mathbf{Var} \left(\sup_{k \geq d+1} \Xi_{j,k} \right) = \mathbf{Var} \left(\sup_{k \geq d+1} \sum_{i=1}^n \chi_{i,k} \right) \leq \sum_{i=1}^n \mathbf{E} \sup_{k \geq d+1} \chi_{i,k}^2 = n \mathbf{E} \sup_{k \geq d+1} \chi_{i,k}^2. \quad (\text{S.11})$$

The term $\mathbf{E} \sup_{k \geq d+1} \chi_{i,k}^2$ can be computed as follows:

$$\begin{aligned} \mathbf{E} \sup_{k \geq d+1} \chi_{i,k}^2 &= \mathbf{E} \sup_{k \geq d+1} [n^{-1} \langle X_i, \psi_j \rangle \langle \mathcal{P}_2 X_i, \psi_k \rangle Z_i]^2 \\ &\leq n^{-2} \mathbf{E} \sup_{k \geq d+1} \|X_i\|^2 \|\mathcal{P}_2 X_i\|^2 \|\psi_j\|^2 \|\psi_k\|^2 Z_i = n^{-2} \mathbf{E} \|X_i\|^2 \|\mathcal{P}_2 X_i\|^2 Z_i. \end{aligned}$$

Since

$$\mathbf{E} \|X_i\|^2 \|\mathcal{P}_2 X_i\|^2 V_i = \int_{S^{d-1}} \int_0^{h_1} \|t\iota_*\theta\|^2 \|t^2 \Pi_x(\theta, \theta)\|^2 f(\exp(t\theta)) t^{d-1} dt d\theta + O(h^{d+8}) = O(h^{d+6}),$$

we apply Lemma S.7 to conclude $\mathbf{E} \|X_i\|^2 \|\mathcal{P}_2 X_i\|^2 Z_i = O(h^{d+6})$. Therefore, $\mathbf{E} \sup_{k \geq d+1} \chi_{i,k}^2 =$

$O(n^{-2}h^{d+6})$. With (S.11), we show that

$$\mathbf{Var} \left(\sup_{k \geq d+1} \Xi_{j,k} \right) = O \left(n^{-1} h^{d+6} \right).$$

Other results are derived in the same way. \square

S.3. Proof of Theorem 4

PROOF OF THEOREM 4. The proof is similar to the proof for Theorem 3. Below we shall only discuss those that are different. Let $h = h_{reg}$ to reduce notational burden.

$$\begin{aligned} \frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{X} &= f(x) \mathbf{v} \kappa_1 \mathbf{v} \\ &+ \begin{bmatrix} O(h) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}}) & O(h^2) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) \\ O(h^2) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) & O(h^3) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+2}) \end{bmatrix} \end{aligned}$$

where

$$\kappa_q = \begin{bmatrix} \kappa_{11,q} & \kappa_{12,q} \\ \kappa_{12,q}^T & \kappa_{22,q} \end{bmatrix}, \kappa_{22,q} = (\kappa_{22,q,j,k})_{j,k=1}^d, \mathbf{v} = \begin{bmatrix} 1 & 0 \\ 0 & h \mathbf{I}_d \end{bmatrix}.$$

Therefore,

$$\begin{aligned} \frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}} &= f(x) \mathbf{v} \kappa_1 \mathbf{v} \\ &+ \begin{bmatrix} O(h) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}}) + O_P(h^{-1-\epsilon d} n^{-\beta}) & O(h^2) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) + O_P(h^{-1-\epsilon d} n^{-\beta}) \\ O(h^2) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) + O_P(h^{-1-\epsilon d} n^{-\beta}) & O(h^3) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}+2}) + O_P(h^{-1-\epsilon d} n^{-\beta}) \end{bmatrix}. \end{aligned}$$

and hence

$$\begin{aligned} \left(\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}} \right)^{-1} &= \mathbf{v}^{-1} \kappa_1^{-1} \mathbf{v}^{-1} / f(x) \\ &+ \begin{bmatrix} O_P(h + h^{-2-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}}) & O_P(1 + h^{-4-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-1}) \\ O_P(1 + h^{-4-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-1}) & O_P(h^{-1} + h^{-5-\epsilon d} n^{-\beta} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-2}) \end{bmatrix}. \end{aligned}$$

This implies that

$$\mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \left\{ (\mathbf{X} - \hat{\mathbf{X}}) \begin{bmatrix} g(x) \\ \nabla g(x) \end{bmatrix} \right\} = \mathbf{e}_1^T \begin{bmatrix} 1 & h^{-1} \\ h^{-1} & h^{-2} \end{bmatrix} O_P(h^{-1-\epsilon d} n^{-\beta}) \mathbf{1}_{d \times 1} = O_P(h^{-1-\epsilon d} n^{-\beta}).$$

By Lemma (S.1), (S.2) and (S.3), one can show that

$$\frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{H} = \begin{bmatrix} h^2 f(x) \int_{\frac{1}{h} \mathbb{D}_x} K(\|\theta\|_{\mathbb{R}^d}) \text{Hess } g(x) \theta d\theta + O_P(h^3 + n^{-1/2} h^{-d/2+2}) \\ h^3 f(x) \int_{\frac{1}{h} \mathbb{D}_x} K(\|\theta\|_{\mathbb{R}^d}) \theta^T \text{Hess } g(x) \theta d\theta + O_P(h^{7/2} + n^{-\frac{1}{2}} h^{-\frac{d}{2}+3}) \end{bmatrix},$$

and hence

$$\frac{1}{n} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \mathbf{H} = \begin{bmatrix} h^2 f(x) \int_{\frac{1}{h} \mathbb{D}_x} K(\|\theta\|_{\mathbb{R}^d}) \text{Hess } g(x) \theta d\theta + O_P(h^3 + n^{-1/2} h^{-d/2+2} + h^{-1-\epsilon d} n^{-\beta}) \\ h^3 f(x) \int_{\frac{1}{h} \mathbb{D}_x} K(\|\theta\|_{\mathbb{R}^d}) \theta^T \text{Hess } g(x) \theta d\theta + O_P(h^{7/2} + n^{-\frac{1}{2}} h^{-\frac{d}{2}+3} + h^{-1-\epsilon d} n^{-\beta}) \end{bmatrix}.$$

Thus, with the choice of h , which implies that $n^{-\frac{1}{2}} h^{-\frac{d}{2}} \ll 1$ and $h^{-1-\epsilon d} n^{-\beta} \ll h^3$,

$$\begin{aligned} \mathbf{e}_1^T (\hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \left\{ \frac{1}{2} \mathbf{H}(x) + O_P(h^3) \right\} &= h^2 \frac{\text{tr}(\text{Hess } g(x) \boldsymbol{\kappa}_{22,1})}{2(\boldsymbol{\kappa}_{11,1} - \boldsymbol{\kappa}_{12,1}^T \boldsymbol{\kappa}_{22,1}^{-1} \boldsymbol{\kappa}_{12,1})} \\ &\quad + O_P(h^{5/2} + n^{-\frac{1}{2}} h^{-\frac{d}{2}+2} + h^{-2-\epsilon d} n^{-\beta}). \end{aligned}$$

Therefore, the conditional bias is

$$\mathbf{E}\{\hat{g}(x) - g(x) \mid \mathcal{D}\} = h^2 \frac{\text{tr}(\text{Hess } g(x) \boldsymbol{\kappa}_{22,1})}{2(\boldsymbol{\kappa}_{11,1} - \boldsymbol{\kappa}_{12,1}^T \boldsymbol{\kappa}_{22,1}^{-1} \boldsymbol{\kappa}_{12,1})} + O_P(h^{5/2} + n^{-\frac{1}{2}} h^{-\frac{d}{2}+2} + h^{-2-\epsilon d} n^{-\beta}).$$

For the conditional variance, by Lemma S.1, S.2 and S.3, we have

$$\frac{1}{n} \mathbf{X}^T \mathbf{W} \mathbf{W} \mathbf{X} = f(x) \mathbf{v} \kappa_2 \mathbf{v} h^{-d} + h^{-d} \begin{bmatrix} O(h) + O_P(n^{-\frac{1}{2}} h^{-\frac{d}{2}}) & O_P(h^2 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) \\ O_P(h^2 + n^{-\frac{1}{2}} h^{-\frac{d}{2}+1}) & O_P(h^{\frac{5}{2}} + n^{-\frac{1}{2}} h^{-\frac{d}{2}+2}) \end{bmatrix}.$$

Thus,

$$\begin{aligned}
& n^{-1} \sigma_\zeta^2 \mathbf{e}_1^T (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} (n^{-1} \mathbf{X}^T \mathbf{W} \mathbf{W} \mathbf{X}) (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \mathbf{e}_1^T \\
&= \frac{1}{nh^d} \frac{\sigma_\varepsilon^2}{f(x)} \mathbf{e}_1^T \kappa_{22,1}^{-1} \kappa_{22,2} \kappa_{22,1}^{-1} \mathbf{e}_1 + O_P \left(n^{-1} h^{-d} (h^{\frac{1}{2}} + n^{-\beta} h^{-4-\epsilon d} + n^{-\frac{1}{2}} h^{-\frac{d}{2}}) \right). \tag{S.12}
\end{aligned}$$

Also, similar to (35), we have

$$\begin{aligned}
& n^{-1} \sigma_\zeta^2 \mathbf{e}_1^T (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \mathbf{1}_{(d+1) \times (d+1)} (n^{-1} \hat{\mathbf{X}}^T \hat{\mathbf{W}} \hat{\mathbf{X}})^{-1} \mathbf{e}_1^T O_P(h^{-d-1-\epsilon d} n^{-\beta}) \\
&= n^{-1} O_P(h^{-2} + n^{-\beta} h^{-5-\epsilon d} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-2}) O_P(h^{-d-1-\epsilon d} n^{-\beta}). \\
&= O_P \left(n^{-1} h^{-d} h^{-1-\epsilon d} n^{-\beta} (h^{-2} + n^{-\beta} h^{-5-\epsilon d} + n^{-\frac{1}{2}} h^{-\frac{d}{2}-2}) \right). \tag{S.13}
\end{aligned}$$

With $n^{-\beta} h^{-2-\epsilon d} \ll h^2$, combining (32), (33), (S.12) and (S.13), we conclude that the conditional variance is

$$\mathbf{Var}\{\hat{g}(x) \mid \mathcal{D}\} = \frac{1}{nh^d} \frac{\sigma_\varepsilon^2}{f(x)} \mathbf{e}_1^T \kappa_{22,1}^{-1} \kappa_{22,2} \kappa_{22,1}^{-1} \mathbf{e}_1 + o_P(n^{-1} h^{-d}).$$

□